



Wave Propagation Methods for Compressible Multicomponent Flow with Moving Interfaces and Boundaries

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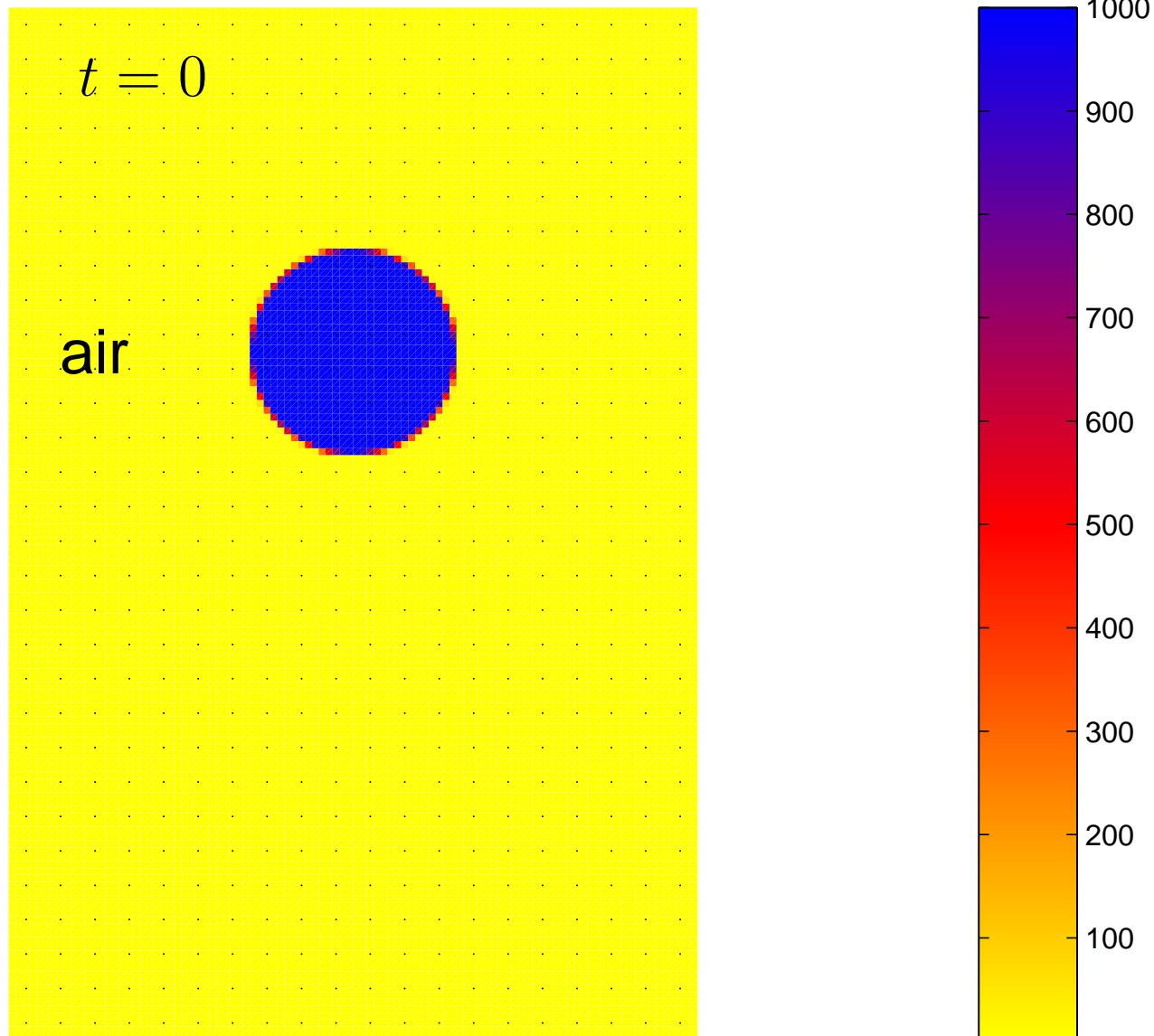
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National Taiwan University

Overview

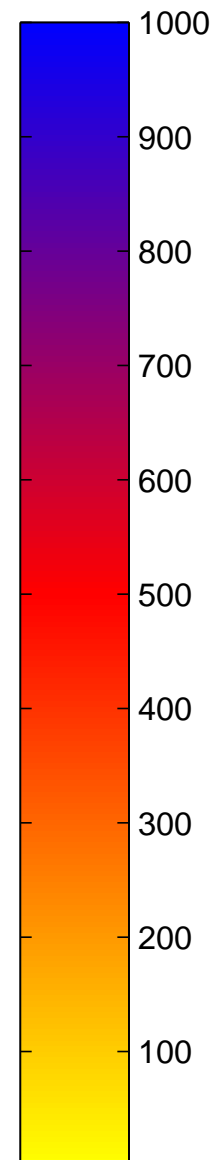
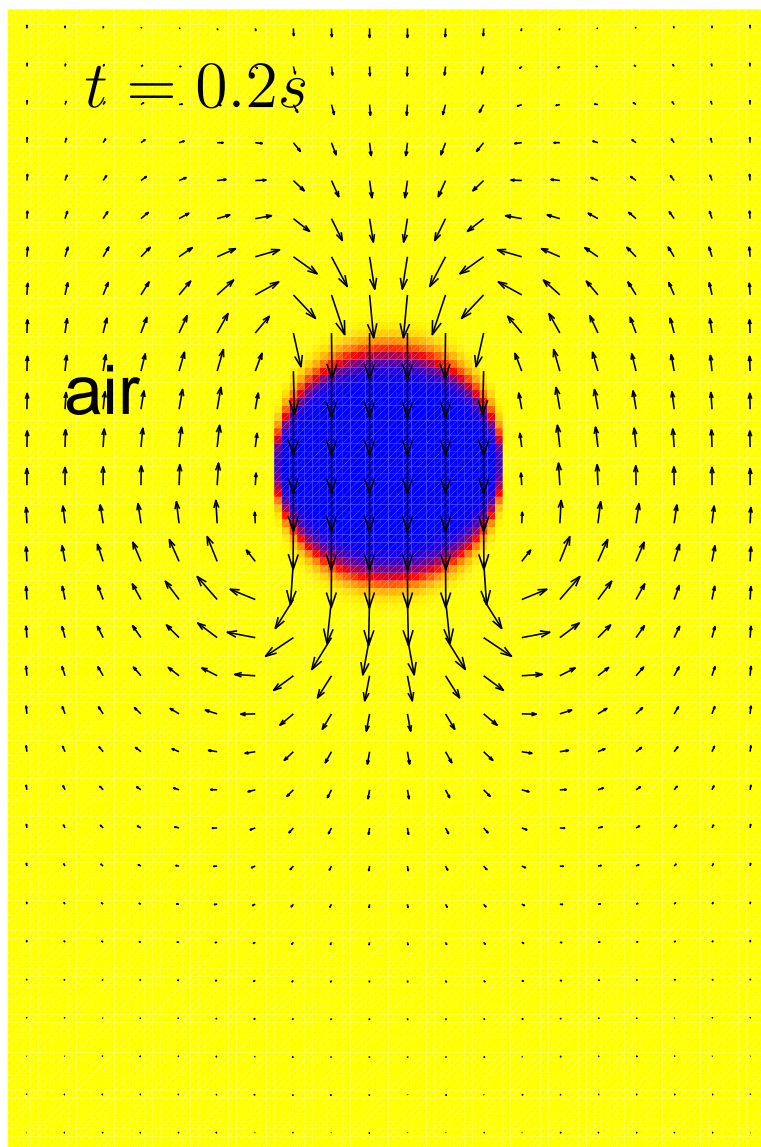


- Illustrative examples
- Mathematical model
 - Fluid-mixture type equations of motion for homogeneous two-phase flow
 - General pressure law for real materials
- Numerical techniques
 - Finite volume method based on wave propagation
 - Surface tracking for moving boundaries
 - Volume tracking for moving interfaces
- Numerical results
- Future work

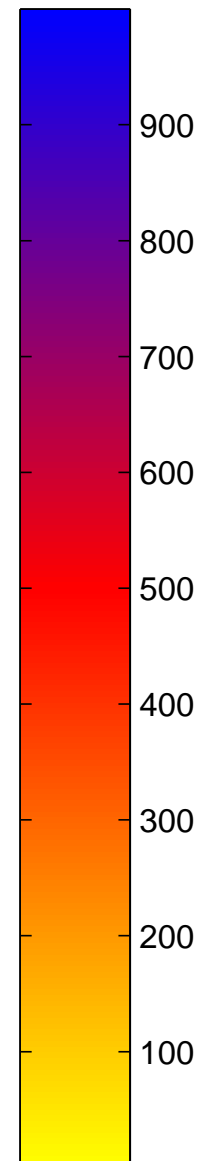
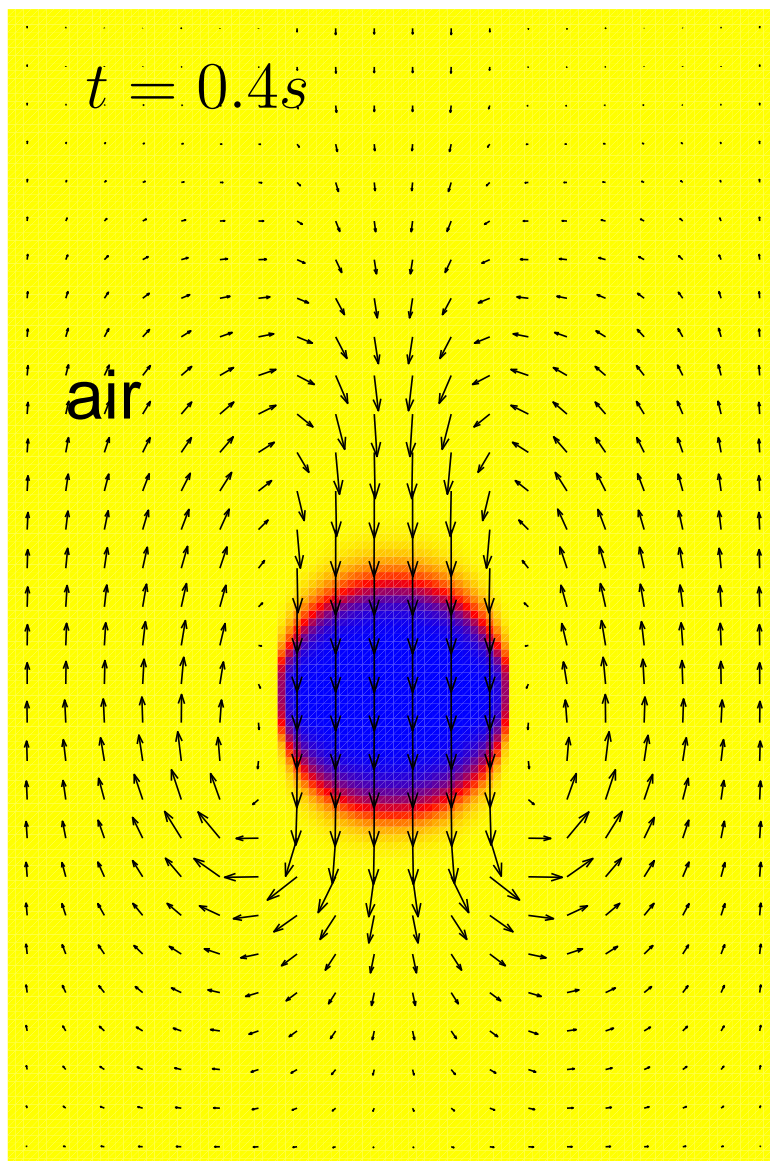
Falling Liquid Drop Problem



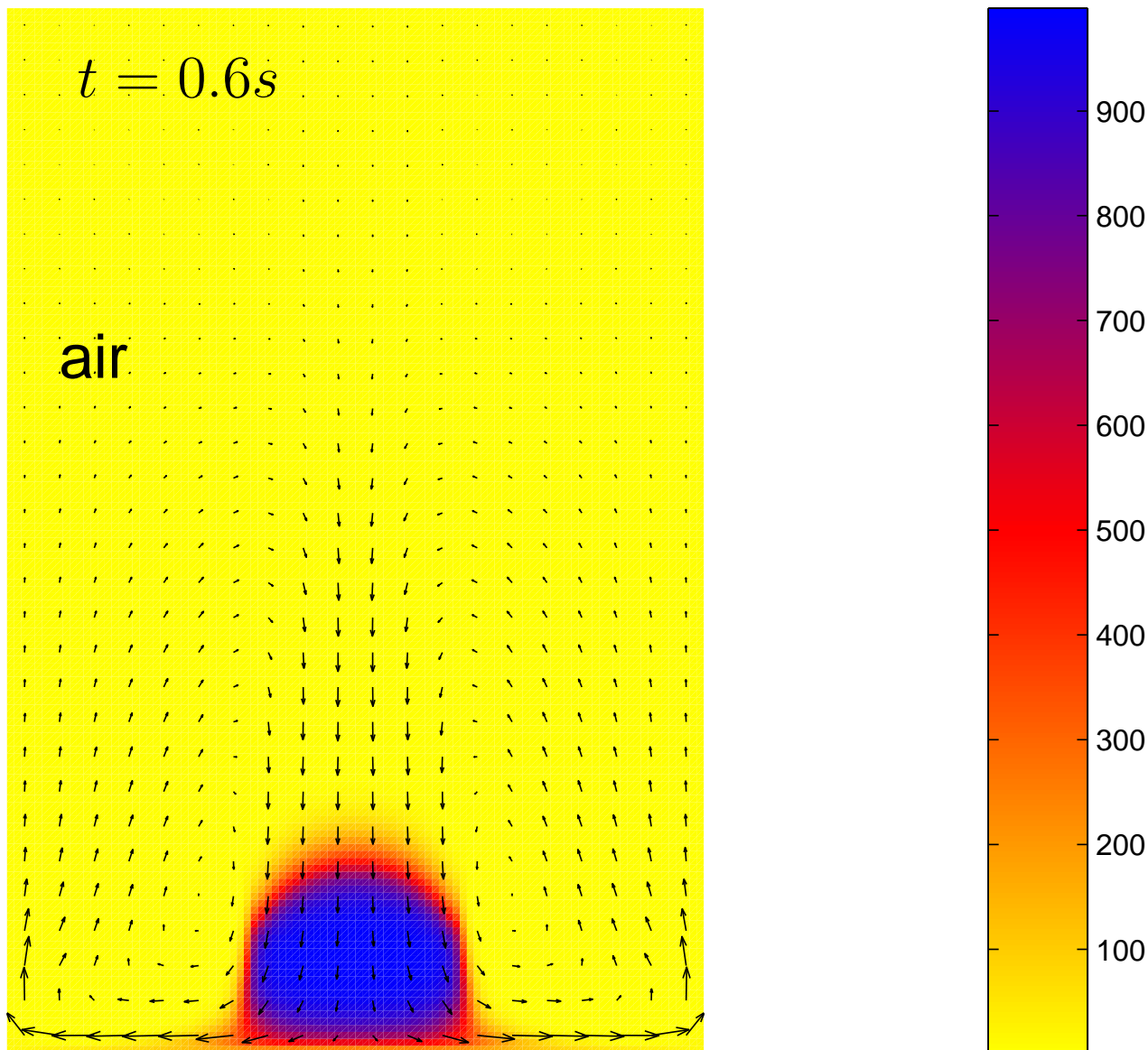
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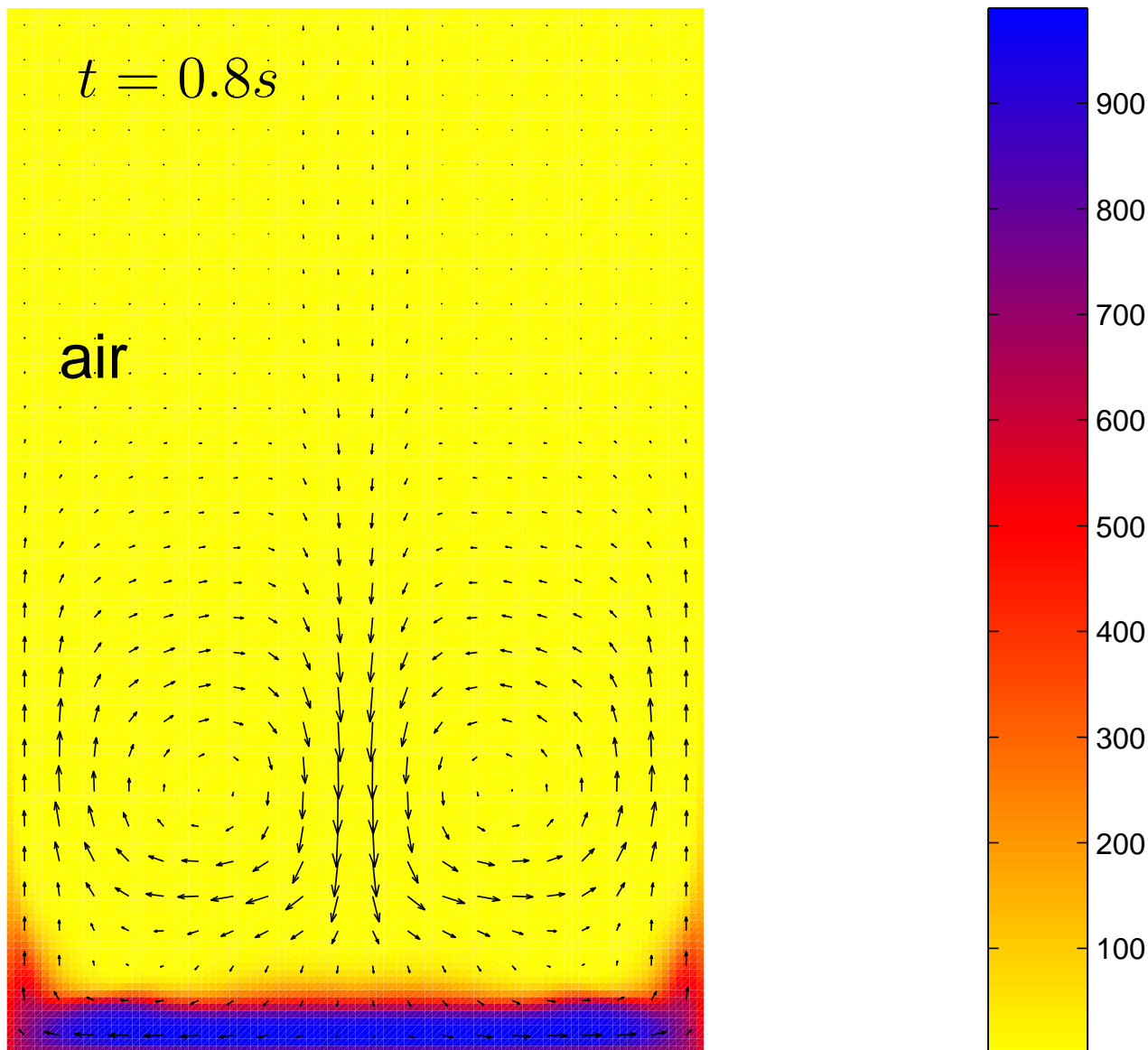
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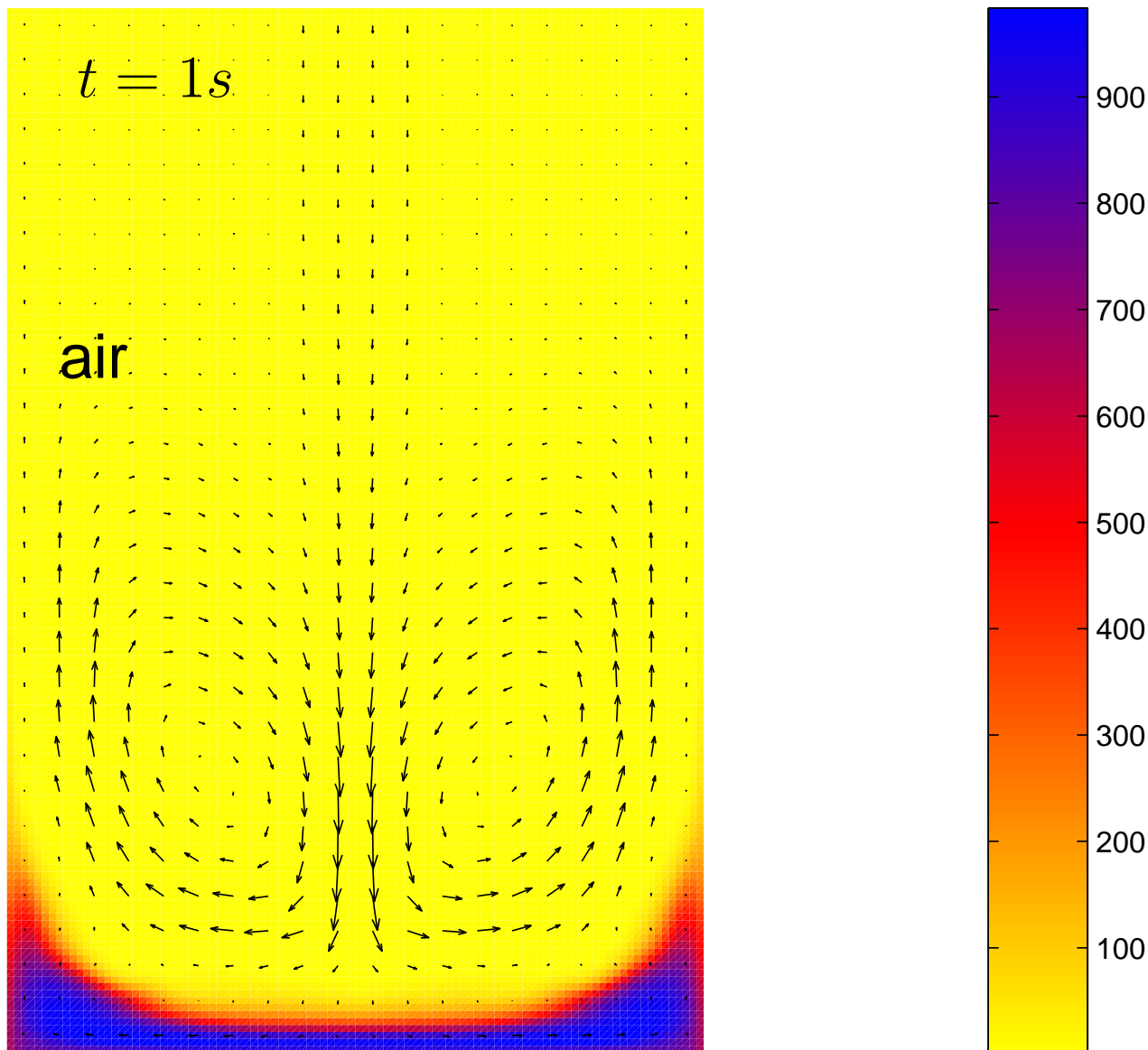
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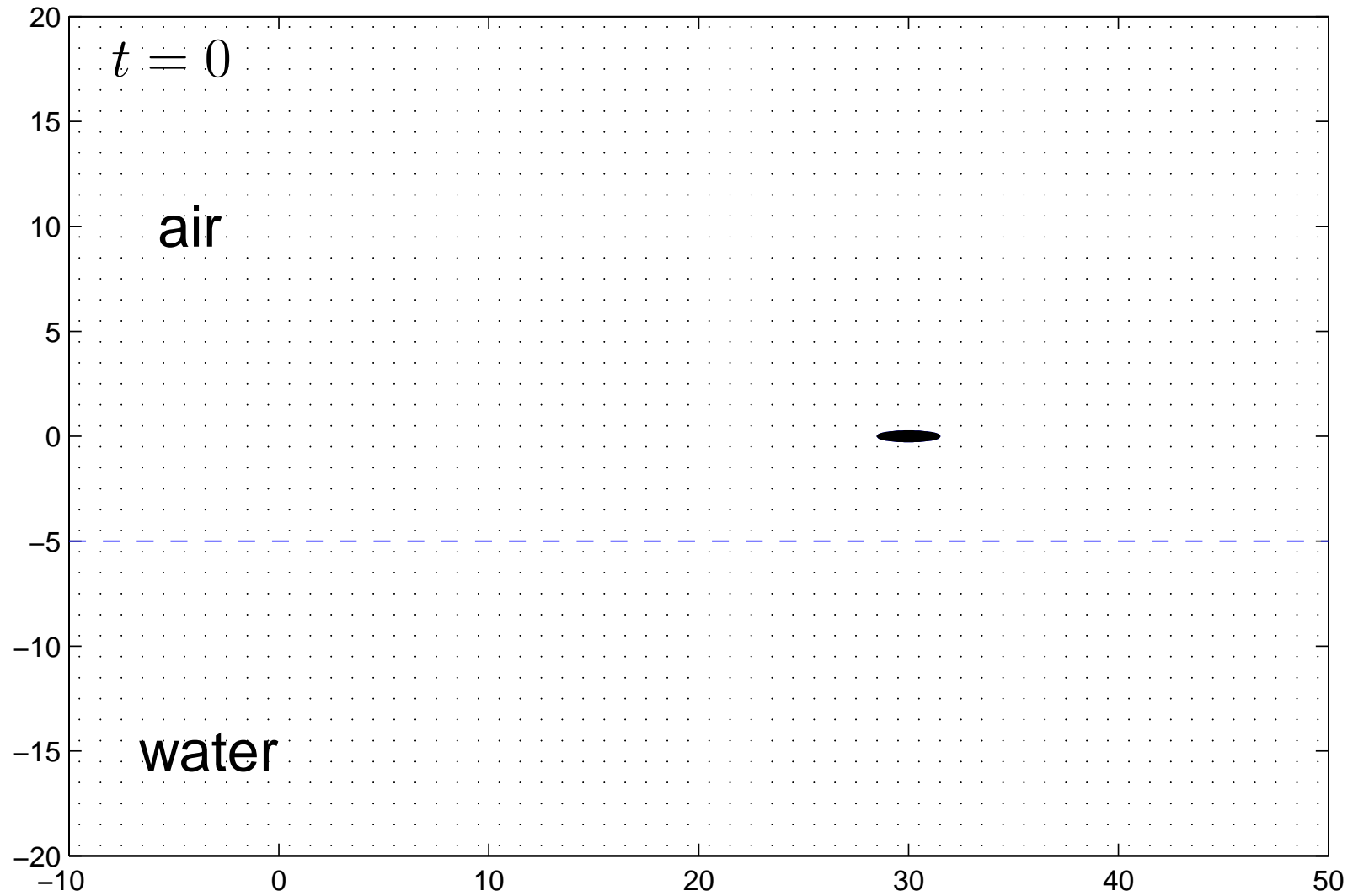
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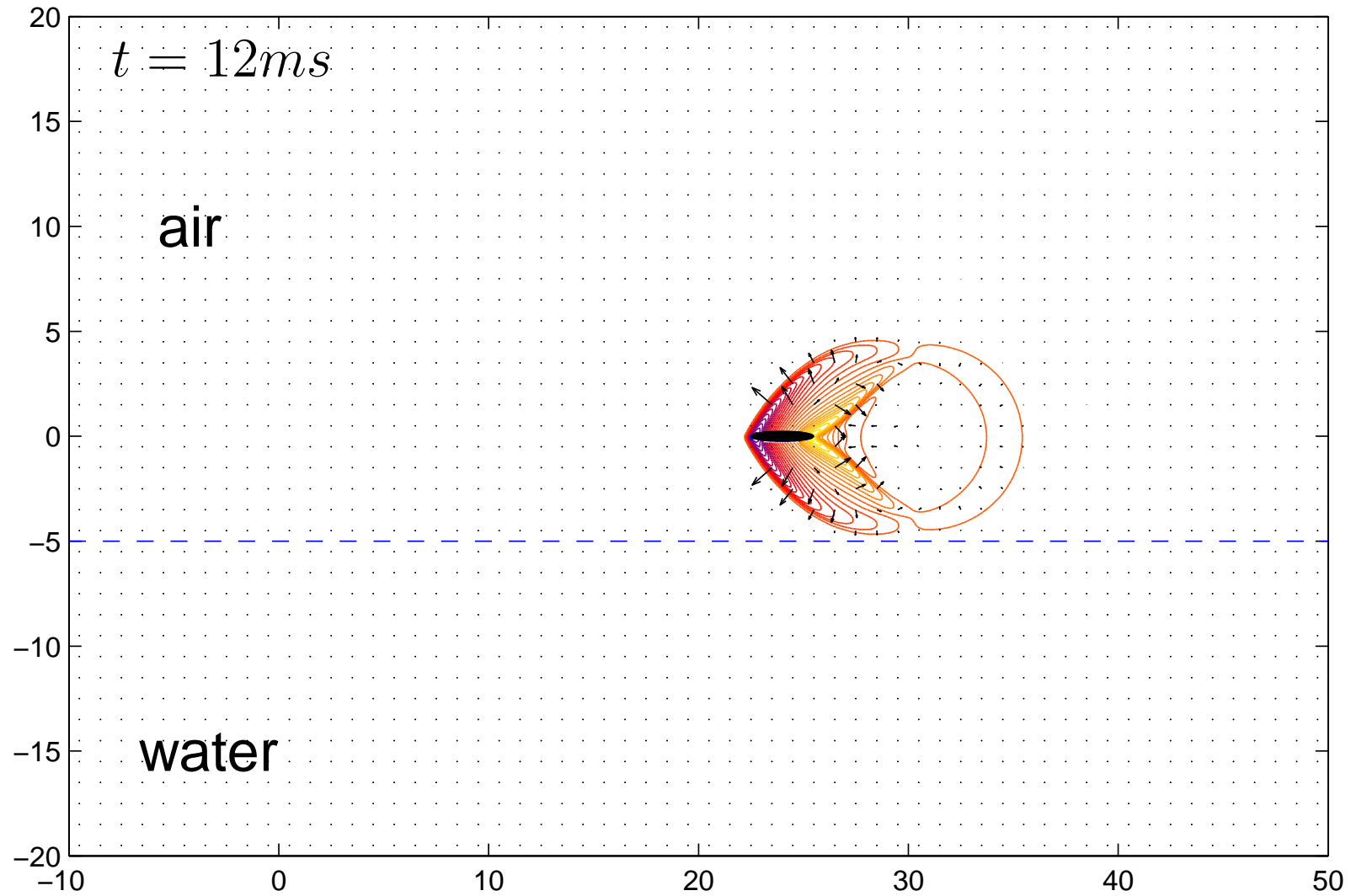
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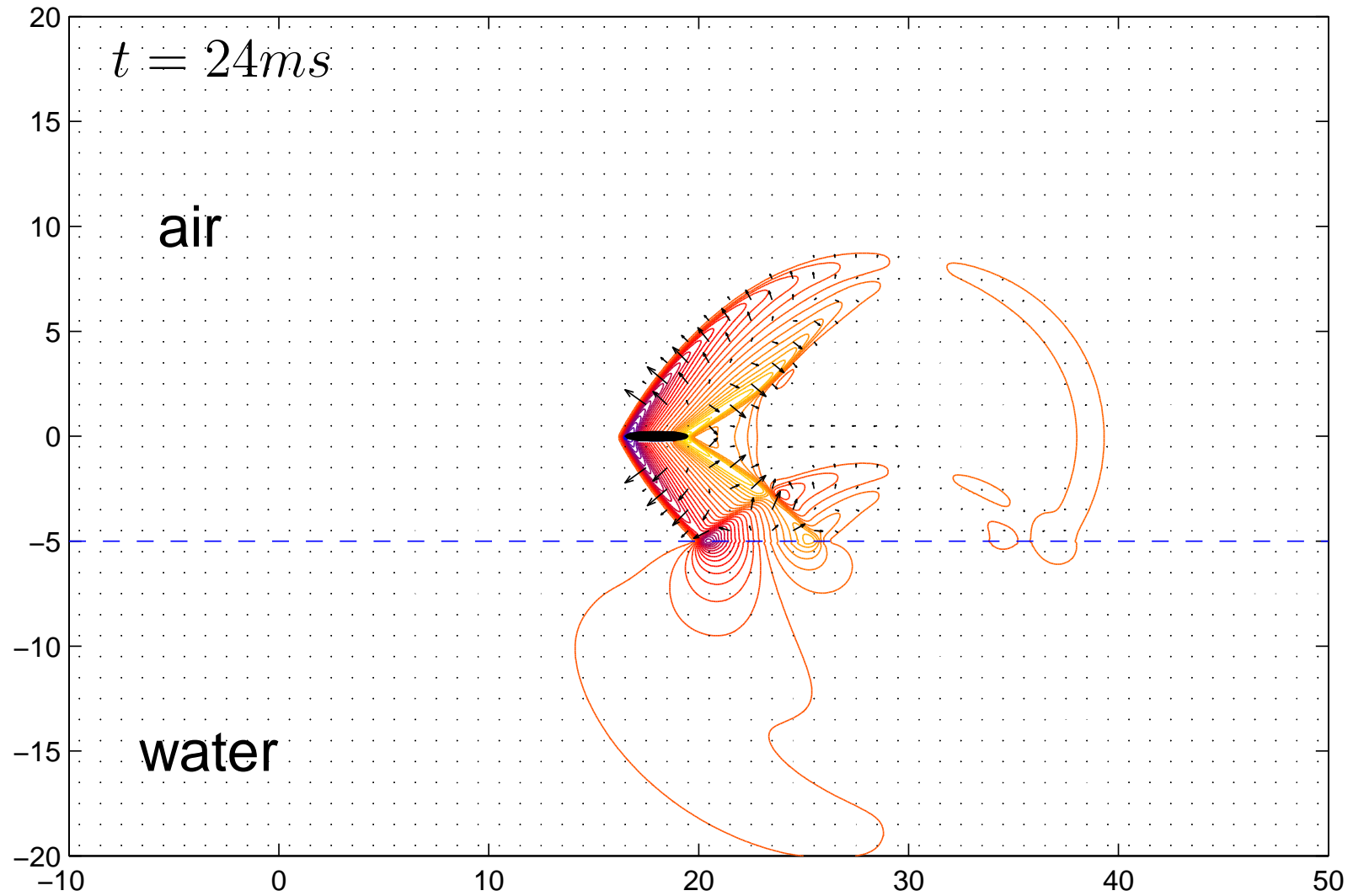
Flying Projectile & Ocean Surface



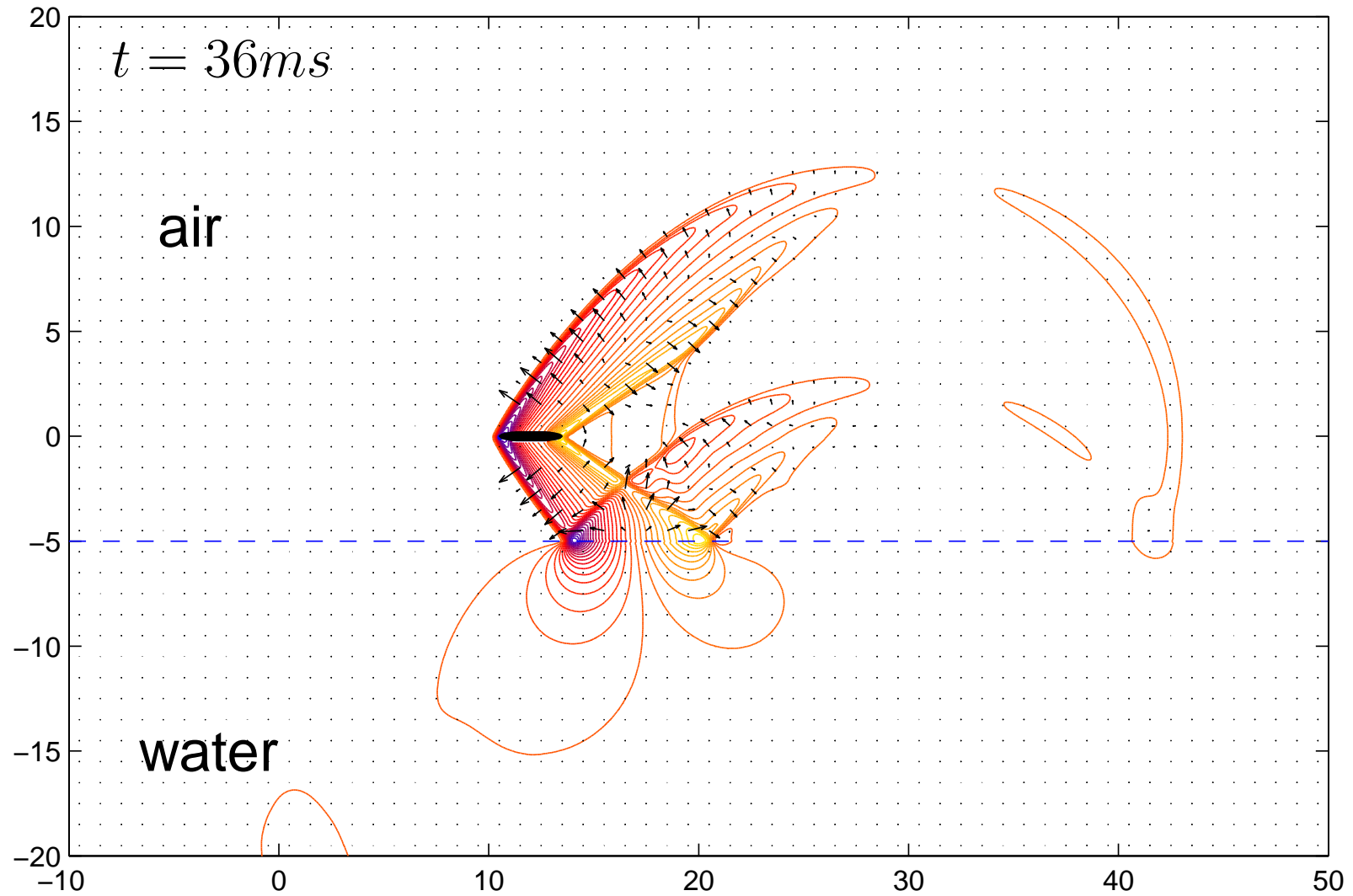
Flying Projectile & Ocean Surface



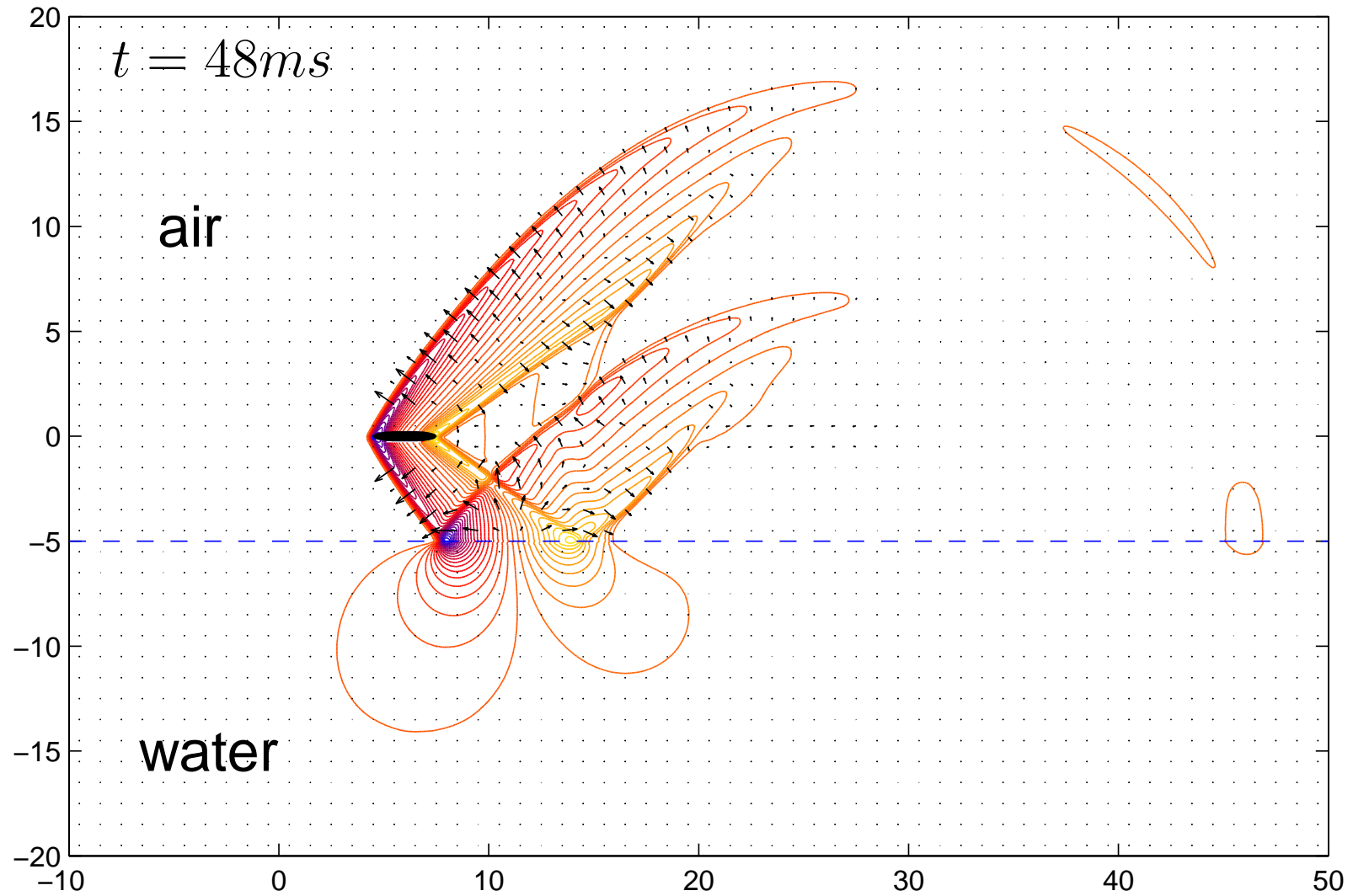
Flying Projectile & Ocean Surface



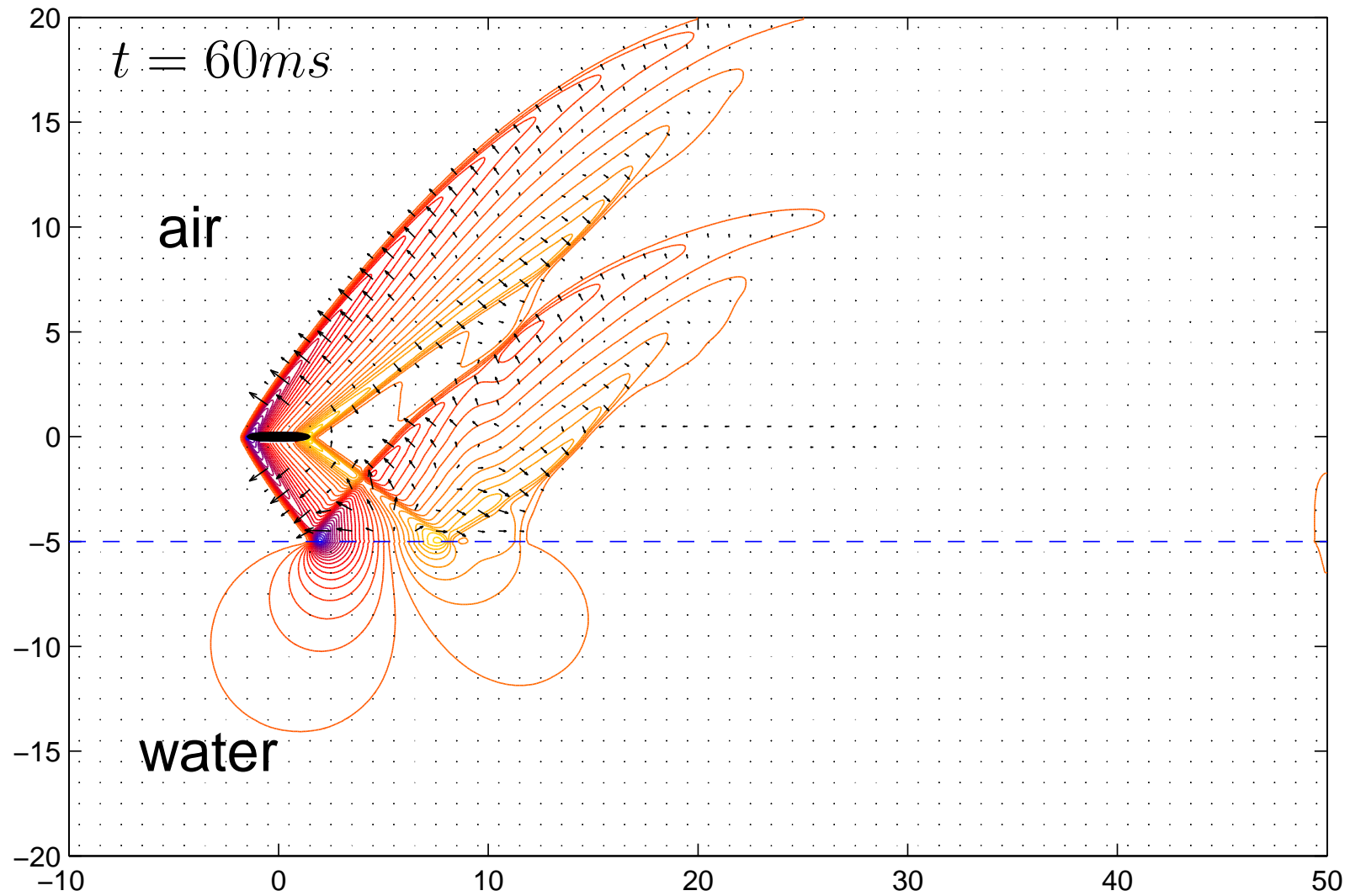
Flying Projectile & Ocean Surface



Flying Projectile & Ocean Surface



Flying Projectile & Ocean Surface



Two Phase Flow Problem



Ignore physical effects such as gravity, viscosity, surface tension, mass diffusion, and so on

Each fluid component satisfies

- Eulerian form **conservation laws**

$$\rho_t + \nabla \cdot (\rho \vec{u}) = 0$$

$$(\rho \vec{u})_t + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = 0$$

$$(\rho E)_t + \nabla \cdot (\rho E \vec{u} + p \vec{u}) = 0$$

- General **pressure law** $p(\rho, e)$

ρ : density, \vec{u} : vector of particle velocity, p : pressure

E : specific total energy, e : specific internal energy

Two-Phase Flow Model



- Model derivation based on **averaging theory** of **Drew** (Theory of Multicomponent Fluids, D.A. Drew & S. L. Passman, Springer, 1999)

Namely, introduce **indicator function** χ_k as

$$\chi_k(M, t) = \begin{cases} 1 & \text{if } M \text{ belongs to phase } k \\ 0 & \text{otherwise} \end{cases}$$

Denote $\langle \psi \rangle$ as **volume averaged** for flow variable ψ ,

$$\langle \psi \rangle = \frac{1}{V} \int_V \psi \, dV$$

Gauss & Leibnitz rules

$$\langle \chi_k \nabla \psi \rangle = \langle \nabla (\chi_k \psi) \rangle - \langle \psi \nabla \chi_k \rangle \quad \& \quad \langle \chi_k \psi_t \rangle = \langle (\chi_k \psi)_t \rangle - \langle \psi (\chi_k)_t \rangle$$

Two-Phase Flow Model (cont.)



Take product of each conservation law with χ_k & perform averaging process. In case of **mass conservation** equation, for example, we have

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot \langle \chi_k \rho_k \vec{u}_k \rangle = \langle \rho_k (\chi_k)_t + \rho_k \vec{u}_k \cdot \nabla \chi_k \rangle$$

Since χ_k is governed by

$$(\chi_k)_t + \vec{u}_0 \cdot \nabla \chi_k = 0 \quad (\vec{u}_0: \text{interface velocity}),$$

this leads to **mass averaged** equation for phase k

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot \langle \chi_k \rho_k \vec{u}_k \rangle = \langle \rho_k (\vec{u}_k - \vec{u}_0) \cdot \nabla \chi_k \rangle$$

Analogously, we may derive averaged equation for **momentum, energy, & entropy** (not shown here)

Two-Phase Flow Model (cont.)



In summary, **averaged** model system, we have, are

$$\langle \chi_k \rho_k \rangle_t + \nabla \cdot \langle \chi_k \rho_k \vec{u}_k \rangle = \langle \rho_k (\vec{u}_k - \vec{u}_0) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rho_k \vec{u}_k \rangle_t + \nabla \cdot \langle \chi_k \rho_k \vec{u}_k \otimes \vec{u}_k \rangle + \nabla \langle \chi_k p_k \rangle = \langle p_k \nabla \chi_k \rangle + \langle \rho_k \vec{u}_k (\vec{u}_k - \vec{u}_0) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rho_k E_k \rangle_t + \nabla \cdot \langle \chi_k \rho_k E_k \vec{u}_k + \chi_k p_k \vec{u}_k \rangle = \langle p_k \vec{u}_k \cdot \nabla \chi_k \rangle + \langle \rho_k E (\vec{u}_k - \vec{u}_0) \cdot \nabla \chi_k \rangle$$

$$\langle \chi_k \rangle_t + \langle \vec{u}_k \cdot \nabla \chi_k \rangle = \langle (\vec{u}_k - \vec{u}_0) \cdot \nabla \chi_k \rangle$$

Note: existence of various **interfacial** source terms
Mathematical as well as **numerical** modelling of these terms
are important (but difficult) for general multiphase flow
problems

Homogeneous 2-Phase Flow Model



- Assume **homogeneous** (1-pressure & 1-velocity) flow; *i.e.*, across interfaces: $p_\iota = p$ & $\vec{u}_\iota = \vec{u}$, $\iota = 0, 1, 2$
- Introduce volume fraction for phase k as $\alpha_k = V_k/V$

Now, by dropping all **interfacial** terms, we may obtain a simplified model as

$$(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \vec{u}) = 0$$

$$(\alpha_k \rho_k \vec{u})_t + \nabla \cdot (\alpha_k \rho_k \vec{u} \otimes \vec{u}) + \nabla (\alpha_k p) = p \nabla \alpha_k$$

$$(\alpha_k \rho_k E_k)_t + \nabla \cdot (\alpha_k \rho_k E_k \vec{u} + \alpha_k p \vec{u}) = p \vec{u} \cdot \nabla \alpha_k$$

$$(\alpha_1)_t + \vec{u} \cdot \nabla \alpha_1 = 0$$

for $k = 1, 2$, & $\alpha_1 + \alpha_2 = 1$. Note this gives $2(2 + N_d) + 1$ equations in total for a N_d -dimension 2-phase flow problem

Homogeneous Flow Model (cont.)



Note that, in practice, rather than using equations $\alpha_k \rho_k \vec{u}$ & $\alpha_k \rho_k E_k$ for each phase, we may write down a system of the form

$$\begin{aligned}(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \vec{u}) &= 0 \\(\rho \vec{u})_t + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p &= 0 \\(\rho E)_t + \nabla \cdot (\rho E \vec{u} + p \vec{u}) &= 0 \\(\alpha_1)_t + \vec{u} \cdot \nabla \alpha_1 &= 0\end{aligned}$$

$$\rho \vec{u} = \sum_{k=1}^2 \alpha_k \rho_k \vec{u}: \text{total momentum}$$

$$\rho E = \sum_{k=1}^2 \alpha_k \rho_k E_k: \text{total energy}$$

This gives $4 + N_d$ equations in total, $N_d + 1$ less than previous model system

Homogeneous Flow Model (cont.)



Note that it is easy to include, for instance, **gravity** & **capillary** effects to the model

$$(\alpha_k \rho_k)_t + \nabla \cdot (\alpha_k \rho_k \vec{u}) = 0 \quad (k = 1, 2)$$

$$(\rho \vec{u})_t + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = \vec{\phi}$$

$$(\rho E)_t + \nabla \cdot (\rho E \vec{u} + p \vec{u}) = \vec{\phi} \cdot \vec{u}$$

$$(\alpha_1)_t + \vec{u} \cdot \nabla \alpha_1 = 0$$

1. Gravity case: $\vec{\phi} = \vec{g}$
2. Capillary case: $\vec{\phi} = \sigma \kappa \nabla \alpha$

\vec{g} : gravitational constant, σ : surface tension coef.

κ : curvature at interface

Homogeneous Flow Model (cont.)



- Mixture equation of state: $p = p(\alpha_2, \alpha_1\rho_1, \alpha_2\rho_2, \rho e)$
- Isobaric closure: $p_1 = p_2 = p$
 - For a class of EOS, **explicit formula** for p is available (examples are given next)
 - For some **complex** EOS, from $(\alpha_2, \rho_1, \rho_2, \rho e)$ in model equations we recover p by solving

$$p_1(\rho_1, \rho_1 e_1) = p_2(\rho_2, \rho_2 e_2) \quad \& \quad \sum_{k=1}^2 \alpha_k \rho_k e_k = \rho e$$

- This homogeneous two-phase model was called **a five-equation model** by Allaire, Clerc, & Kokh (JCP 2002) or **a volume-fraction model** by Shyue (JCP 1998)

Homogeneous Flow Model (cont.)



- **Polytropic ideal gas:** $p_k = (\gamma_k - 1)\rho_k e_k$

$$\rho e = \sum_{k=1}^2 \alpha_k \rho_k e_k = \sum_{k=1}^2 \alpha_k \frac{p}{\gamma_k - 1} \quad \Rightarrow$$

$$p = \rho e / \sum_{k=1}^2 \frac{\alpha_k}{\gamma_k - 1}$$

Homogeneous Flow Model (cont.)



- **Polytropic ideal gas:** $p_k = (\gamma_k - 1)\rho_k e_k$

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$$p = \rho e / \sum_{k=1}^2 \frac{\alpha_k}{\gamma_k - 1}$$

- **Van der Waals gas:** $p_k = \left(\frac{\gamma_k - 1}{1 - b_k \rho_k}\right)(\rho_k e_k + a_k \rho_k^2) - a_k \rho_k^2$

$$\rho e = \sum_{k=1}^2 \alpha_k \rho_k e_k = \sum_{k=1}^2 \alpha_k \left[\left(\frac{1 - b_k \rho_k}{\gamma_k - 1}\right) (p + a_k \rho_k^2) - a_k \rho_k^2 \right] \quad \Rightarrow$$

$$p = \left[\rho e - \sum_{k=1}^2 \alpha_k \left(\frac{1 - b_k \rho_k}{\gamma_k - 1} - 1 \right) a_k \rho_k^2 \right] / \sum_{k=1}^2 \alpha_k \left(\frac{1 - b_k \rho_k}{\gamma_k - 1} \right)$$

Homogeneous Flow Model (cont.)



- **Two-molecular vibrating gas:** $p_k = \rho_k R_k T(e_k)$, T satisfies

$$e = \frac{RT}{\gamma - 1} + \frac{RT_{\text{vib}}}{\exp(T_{\text{vib}}/T) - 1}$$

As before, we now have

$$\begin{aligned} \rho e &= \sum_{k=1}^2 \alpha_k \rho_k e_k = \sum_{k=1}^2 \alpha_k \left[\left(\frac{\rho_k R_k T_k}{\gamma_k - 1} \right) + \frac{\rho_k R_k T_{\text{vib},k}}{\exp(T_{\text{vib},k}/T_k) - 1} \right] \\ &= \sum_{k=1}^2 \alpha_k \left[\left(\frac{p}{\gamma_k - 1} \right) + \frac{p_{\text{vib},k}}{\exp(p_{\text{vib},k}/p) - 1} \right] \quad (\text{Nonlinear eq.}) \end{aligned}$$

Homogeneous Flow Model (cont.)



- It is easy to show **entropies**, S_k , $k = 1, 2$, satisfy

$$\left(\frac{\partial p_1}{\partial S_1}\right)_{\rho_1} \frac{DS_1}{Dt} - \left(\frac{\partial p_2}{\partial S_2}\right)_{\rho_2} \frac{DS_2}{Dt} = (\rho_1 c_1^2 - \rho_2 c_2^2) \nabla \cdot \vec{u}$$

Homogeneous Flow Model (cont.)



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- Murrone & Guillard** (JCP 2005) proposed a **reduced** two-phase flow model in which

$$(\alpha_1)_t + \vec{u} \cdot \nabla \alpha_1 = \alpha_1 \alpha_2 \left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\sum_{k=1}^2 \alpha_k \rho_k c_k^2} \right)$$

and now **entropy** of each phase satisfy

$$\frac{DS_k}{Dt} = \frac{\partial S_k}{\partial t} + \vec{u} \cdot \nabla S_k = 0, \quad \text{for } k = 1, 2$$

Some Remarks



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3. In the model, it is **not** at all clear on how to compute **nonlinear** term ρ^ν , $\nu > 1$ from α_k & $\alpha_k\rho_k$
4. In fact, there are **other** set of **model systems** proposed in the literature that are more robust for homogeneous flow & in other more complicated context (examples)
5. In cases when individual **pressure law** differs in form (see below), **new** mixture pressure law should be devised first & **construct** model equations based on that

Barotropic & Non-Barotropic Flow



- Fluid component 1: **Tait** EOS

$$p(\rho) = (p_0 + \mathcal{B}) \left(\frac{\rho}{\rho_0} \right)^\gamma - \mathcal{B}$$

- Fluid component 2: **Noble-Abel** EOS

$$p(\rho, e) = \left(\frac{\gamma - 1}{1 - b\rho} \right) \rho e$$

- **Mixture** pressure law (Shyue, Shock Waves 2006)

$$p = \begin{cases} (p_0 + \mathcal{B}) \left(\frac{\rho}{\rho_0} \right)^\gamma - \mathcal{B} & \text{if } \alpha = 1 \\ \left(\frac{\gamma - 1}{1 - b\rho} \right) (\rho e - \mathcal{B}) - \mathcal{B} & \text{if } \alpha \neq 1 \end{cases}$$

Barotropic Two-Phase Flow



- Fluid component ι : **Tait** EOS

$$p(\rho) = (p_{0\iota} + \mathcal{B}_\iota) \left(\frac{\rho}{\rho_{0\iota}} \right)^{\gamma_\iota} - \mathcal{B}_\iota, \quad \iota = 1, 2$$

- **Mixture** pressure law (Shyue, JCP 2004)

$$p = \begin{cases} (p_{0\iota} + \mathcal{B}_\iota) \left(\frac{\rho}{\rho_{0\iota}} \right)^{\gamma_\iota} - \mathcal{B}_\iota & \text{if } \alpha = \alpha_\iota \text{ (0 or 1)} \\ (\gamma - 1) \rho \left(e + \frac{\mathcal{B}}{\rho_0} \right) - \gamma \mathcal{B} & \text{if } \alpha \in (0, 1) \end{cases}$$

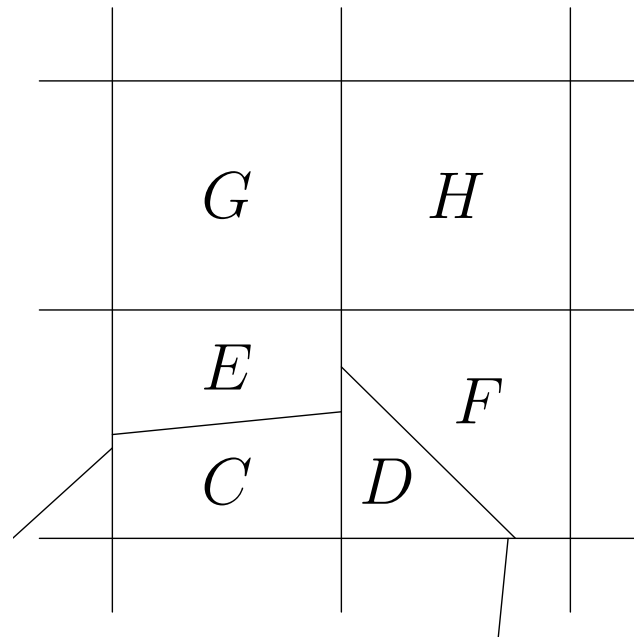
Wave Propagation Method



Finite volume formulation of wave propagation method, Q_S^n gives **approximate** value of **cell average** of solution q over cell S at time t_n

$$Q_S^n \approx \frac{1}{\mathcal{M}(S)} \int_S q(X, t_n) dV$$

$\mathcal{M}(S)$: measure (**area** in 2D or **volume** in 3D) of cell S

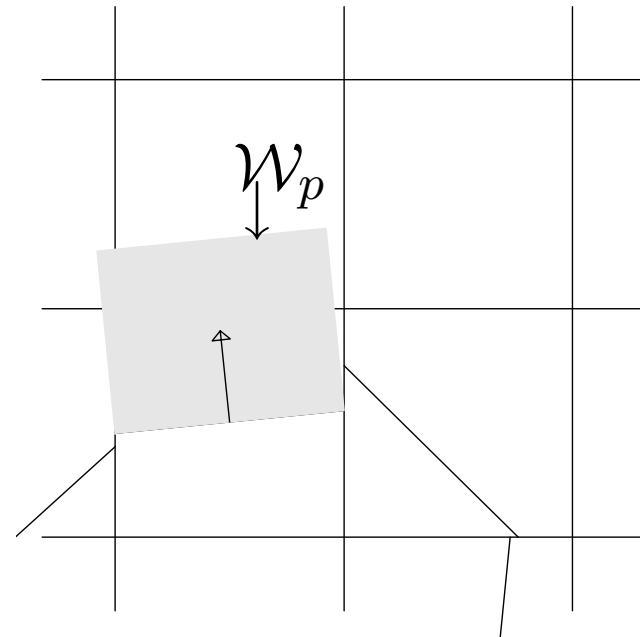
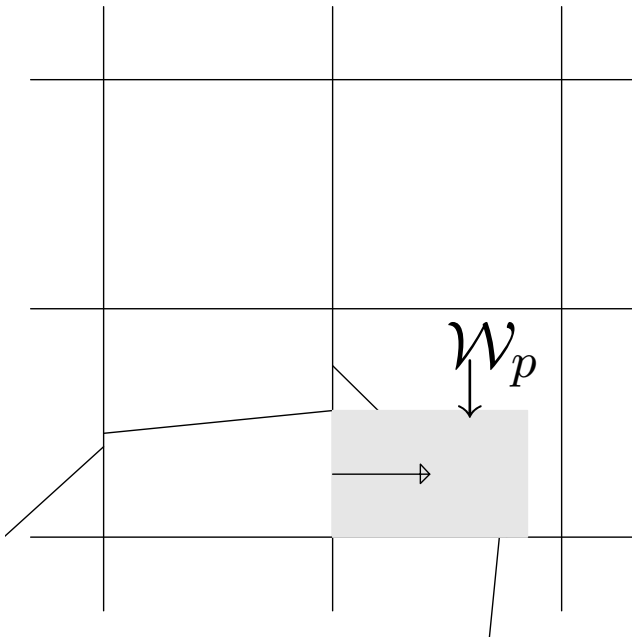


Wave Propagation Method (cont.)



- First order version: **Piecewise constant** wave update
 - Godunov-type method: Solve **Riemann problem** at each cell interface in **normal** direction & use resulting **waves** to update cell averages

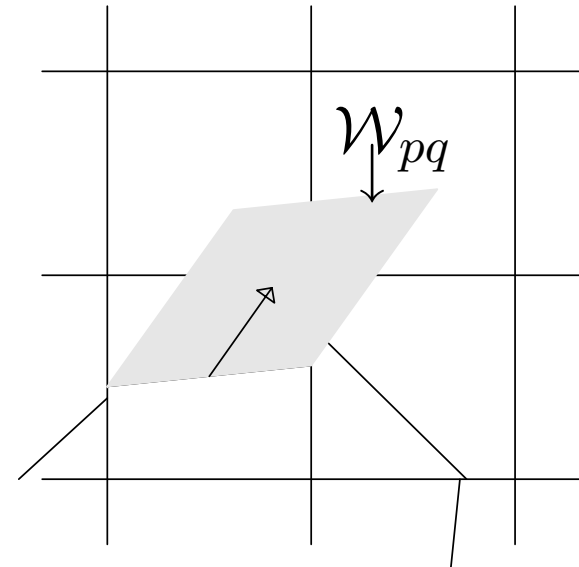
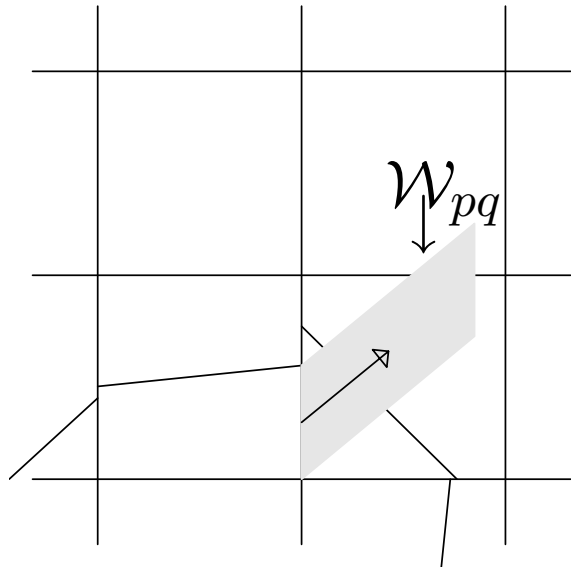
$$Q_S^{n+1} := Q_S^{n+1} - \frac{\mathcal{M}(\mathcal{W}_p \cap S)}{\mathcal{M}(S)} R_p, \quad R_p \text{ being jump from RP}$$



Wave Propagation Method (cont.)



- First order version: **Transverse-wave** included
 - Use transverse portion of equation, solve **Riemann problem** in **transverse** direction, & use resulting waves to update cell averages as usual
 - **Stability** of method is typically improved, while **conservation** of method is maintained

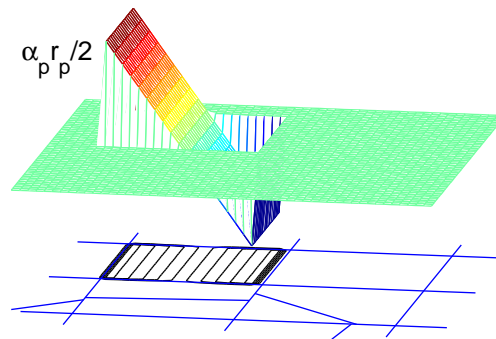


Wave Propagation Method (cont.)

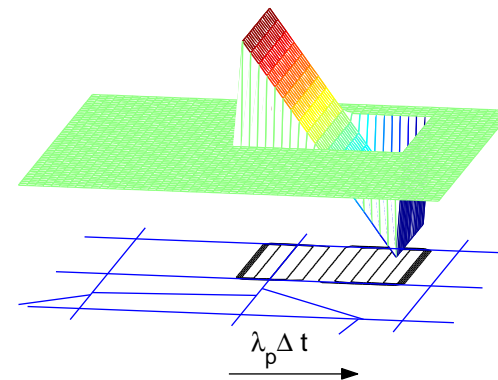


- High resolution version: **Piecewise linear** wave update
wave **before** propagation **after** propagation

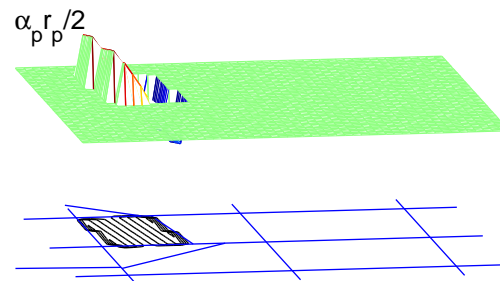
a)



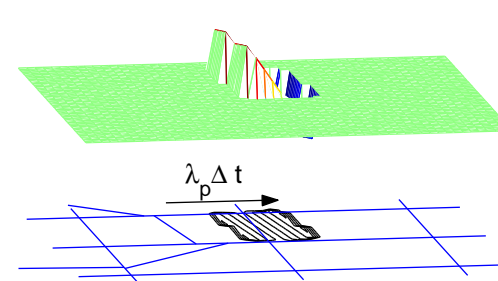
b)



c)



d)



Volume Tracking Algorithm



1. Volume moving procedure

(a) Volume fraction update

Take a time step on current grid to update cell averages of volume fractions at next time step

(b) Interface reconstruction

Find new interface location based on volume fractions obtained in (a) using an interface reconstruction scheme. Some cells will be subdivided & values in each subcell must be initialized.

2. Physical solution update

Take same time interval as in (a), but use a method to update cell averages of multicomponent model on new grid created in (b)

Interface Reconstruction Scheme



Given **volume fractions** on current grid, piecewise linear interface reconstruction (PLIC) method does:

1. Compute **interface normal**

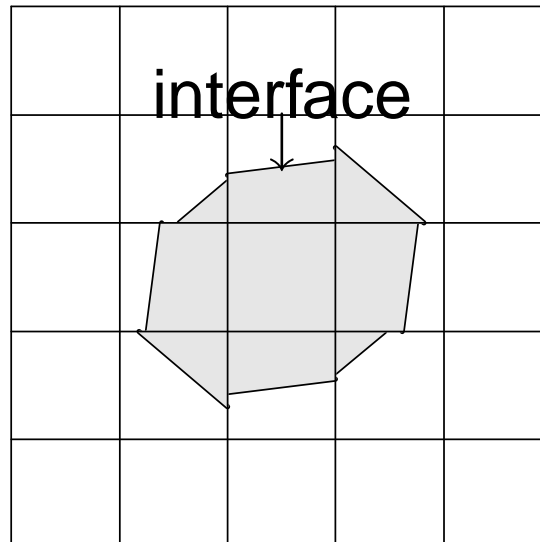
- **Gradient** method of Parker & Youngs
- **Least squares** method of Puckett

2. Determine **interface location** by **iterative bisection**

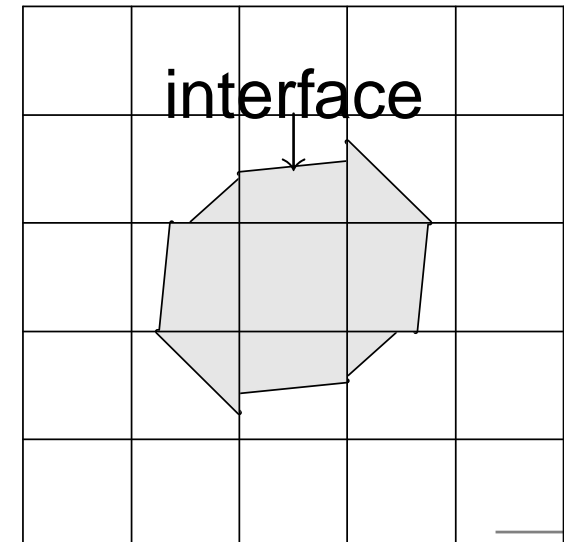
Data set

0	0	0	0	0
0	0.09	0.51	0.29	0
0	0.68	1	0.68	0
0	0.29	0.51	0.09	0
0	0	0	0	0

Parker & Youngs



Puckett



Volume Moving Procedure

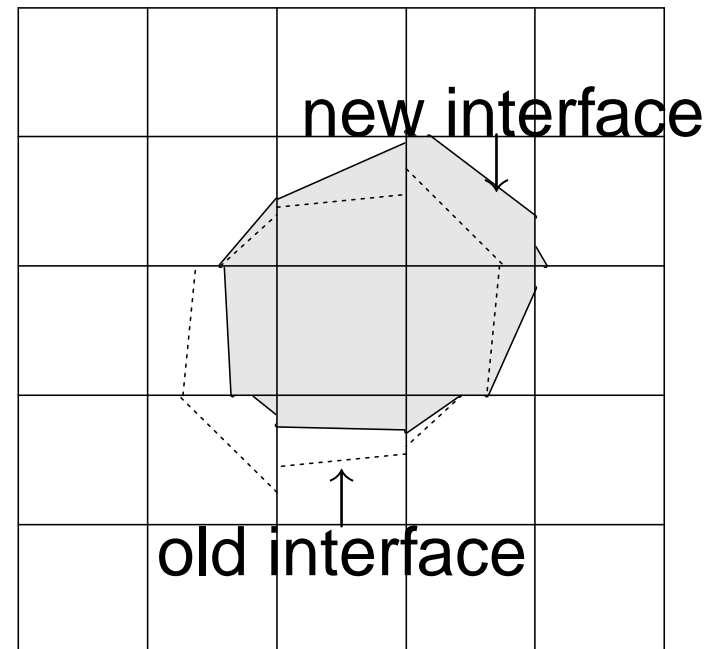


- (a) Volume fractions given in previous slide are updated with uniform $(u, v) = (1, 1)$ over $\Delta t = 0.06$
- (b) New interface location is reconstructed

(a)

0	0	0	1(-3)	0
0	0.11	0.72	0.74	5(-3)
0	0.38	1	0.85	0
0	0.01	0.25	0.06	0
0	0	0	0	0

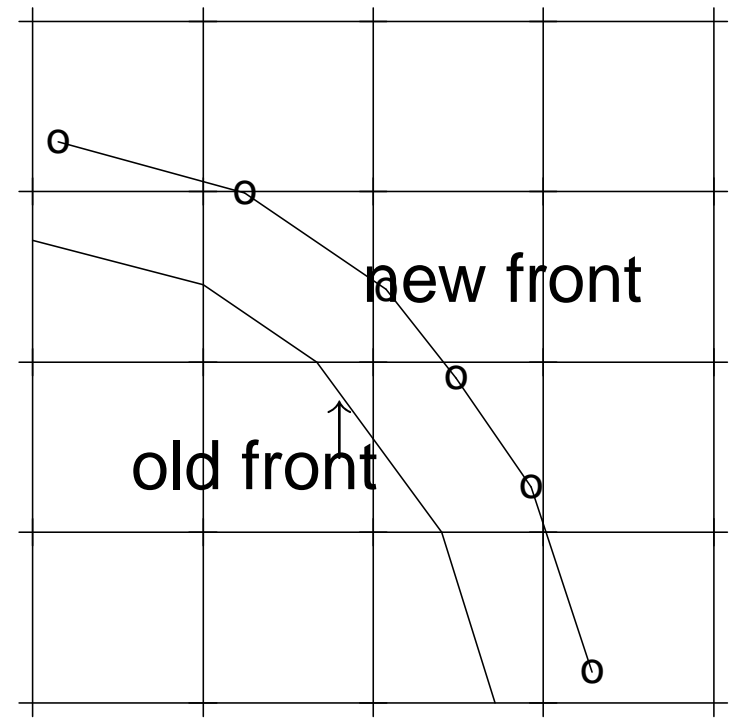
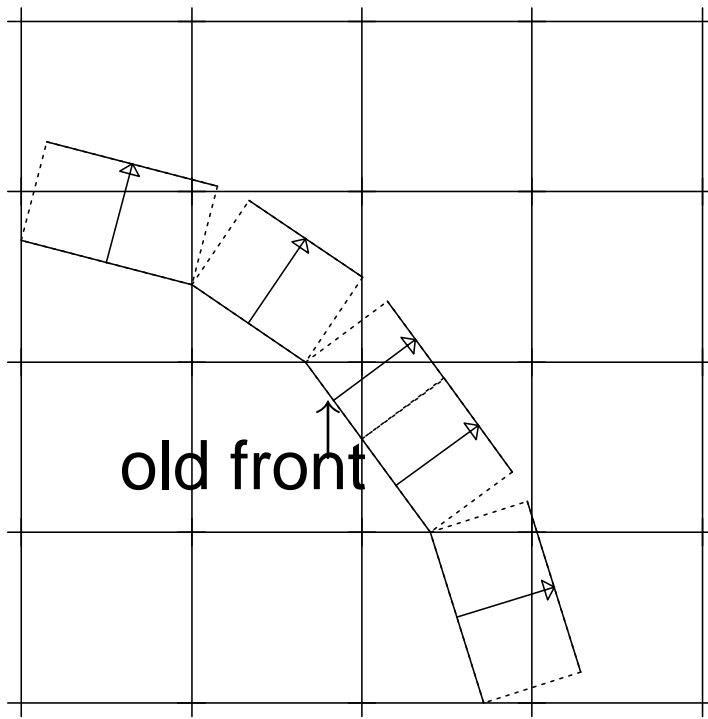
(b)



Surface Moving Procedure



Solve Riemann problem at tracked interfaces & use resulting wave speed of the tracked wave family over Δt to find new location of interface at the next time step



Boundary Conditions

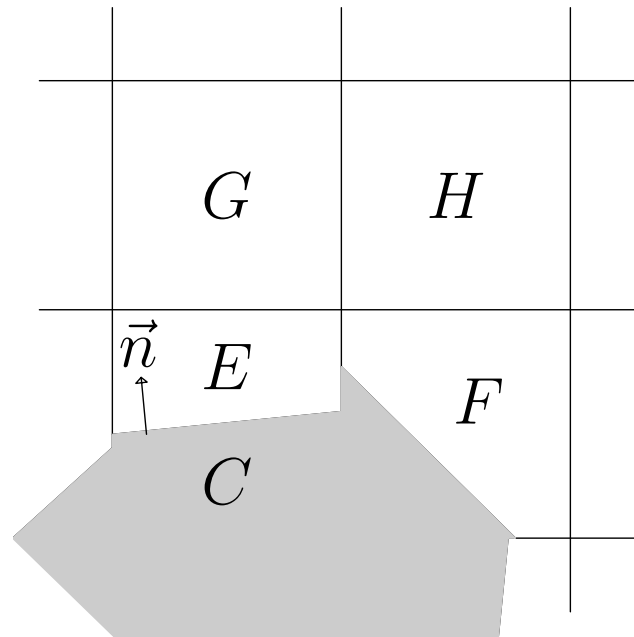


For tracked segments representing **rigid** (solid wall) boundary (stationary or moving), **reflection principle** is used to assign states for **fictitious subcells** in each time step:

$$z_C := z_E \quad (z = \rho, p, \alpha)$$

$$\vec{u}_C := \vec{u}_E - 2(\vec{u}_E \cdot \vec{n})\vec{n} + 2(\vec{u}_0 \cdot \vec{n})$$

\vec{u}_0 : moving boundary velocity



Interface Conditions



For tracked segments representing **material interfaces**, **pressure equilibrium** as well as **velocity continuity** conditions across interfaces are **fulfilled** by

1. Devise of the wave-propagation method
2. Choice of Riemann solver used in the method

Stability Issues

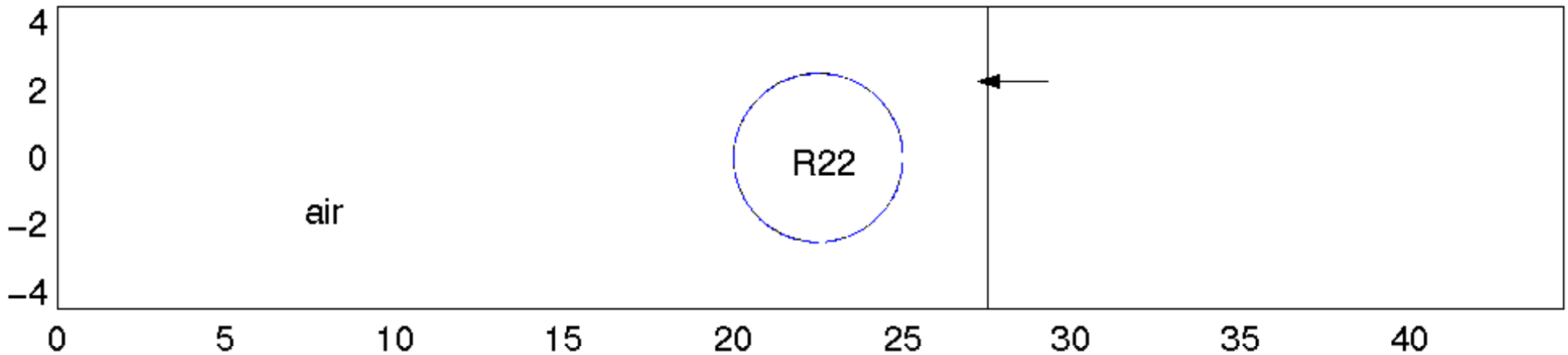


- Choose time step Δt based on uniform grid mesh size $\Delta x, \Delta y$ as

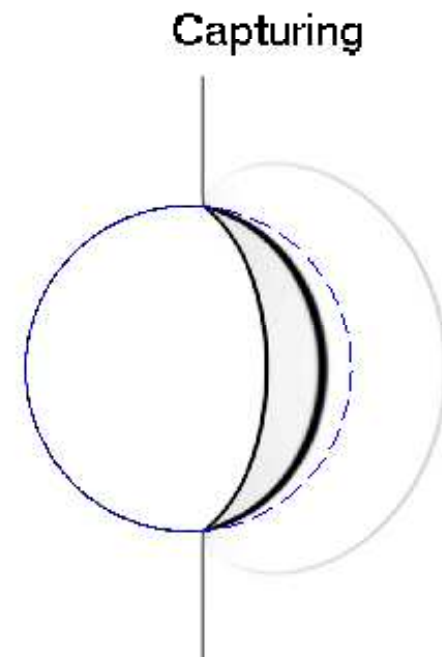
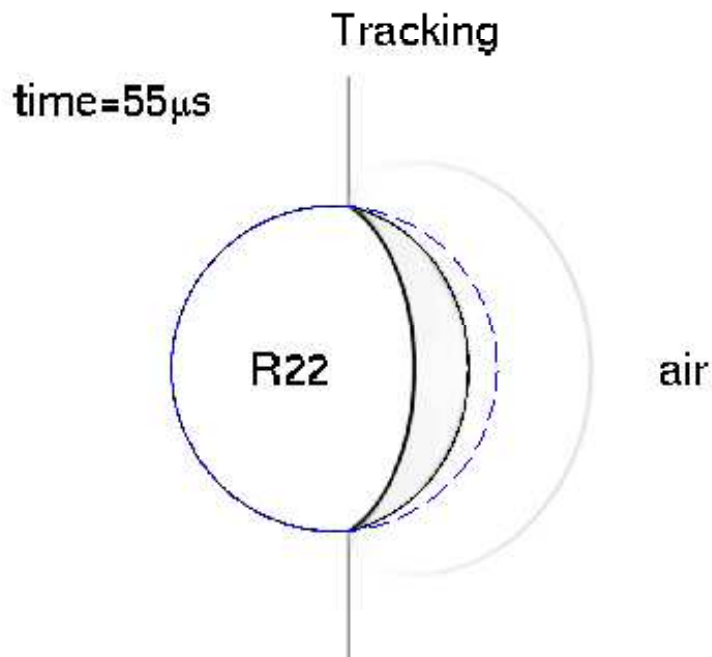
$$\frac{\Delta t \max_{p,q} (\lambda_p, \mu_q)}{\min(\Delta x, \Delta y)} \leq 1,$$

- λ_p, μ_q : speed of p -wave, q -wave from Riemann problem solution in normal-, transverse-directions
- Use **large time step** method of LeVeque (*i.e.*, **wave interactions** are assumed to behave in **linear** manner) to maintain **stability** of method even in the presence of small Cartesian cut cells
- Apply **smoothing** operator (such as, h -box approach of Berger *et al.*) locally for cell averages in irregular cells

Shock-Bubble Interaction Problem



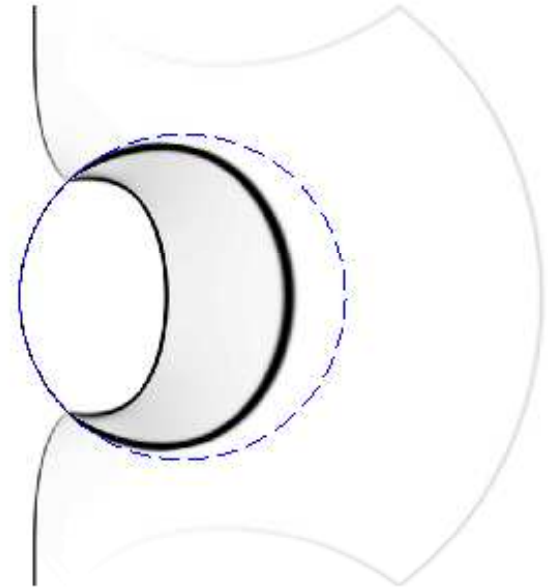
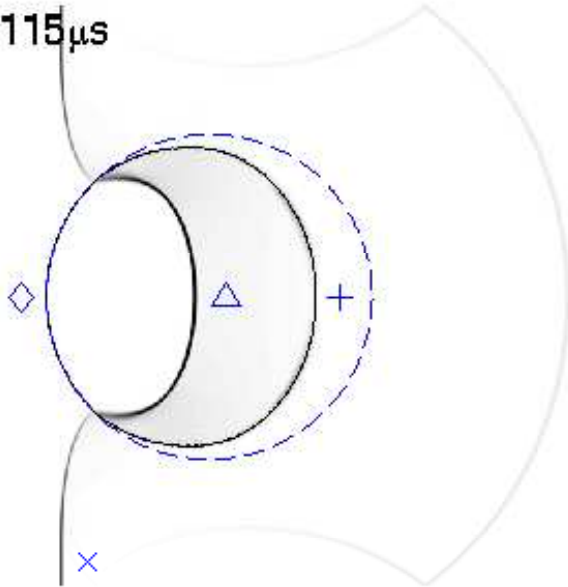
Shock-Bubble Interaction Problem



Shock-Bubble Interaction Problem



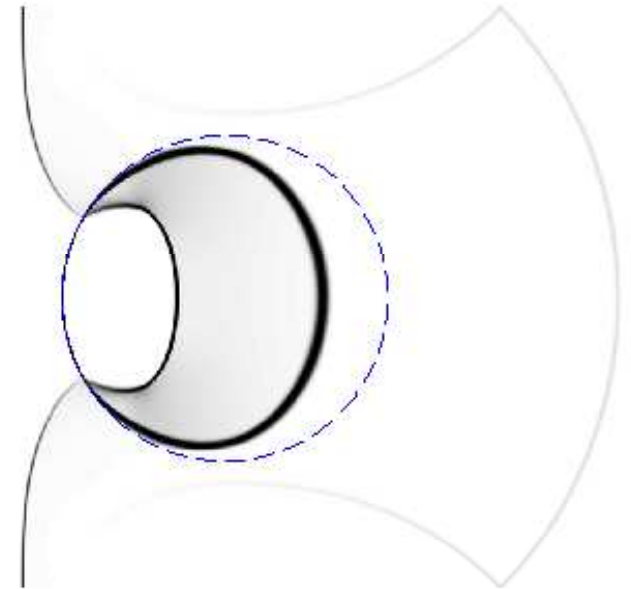
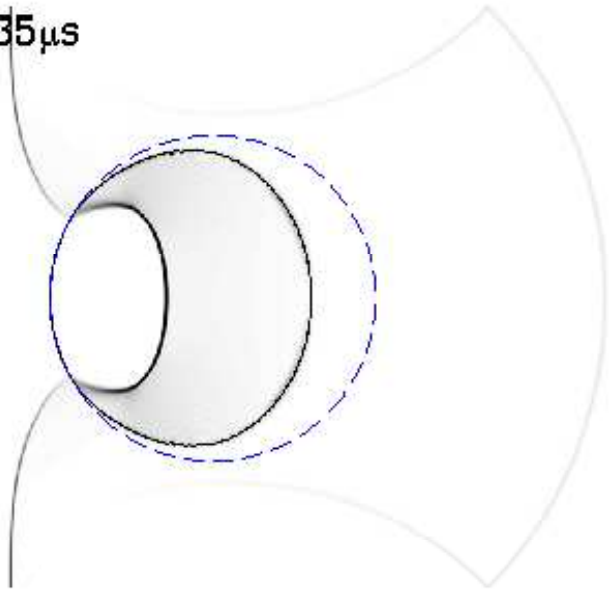
time = 115 μ s



Shock-Bubble Interaction Problem



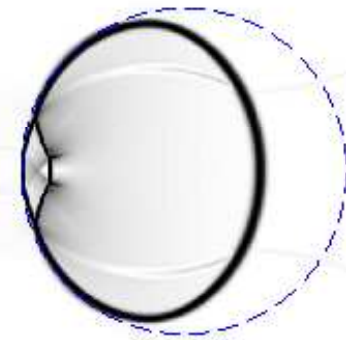
time = 135 μ s



Shock-Bubble Interaction Problem



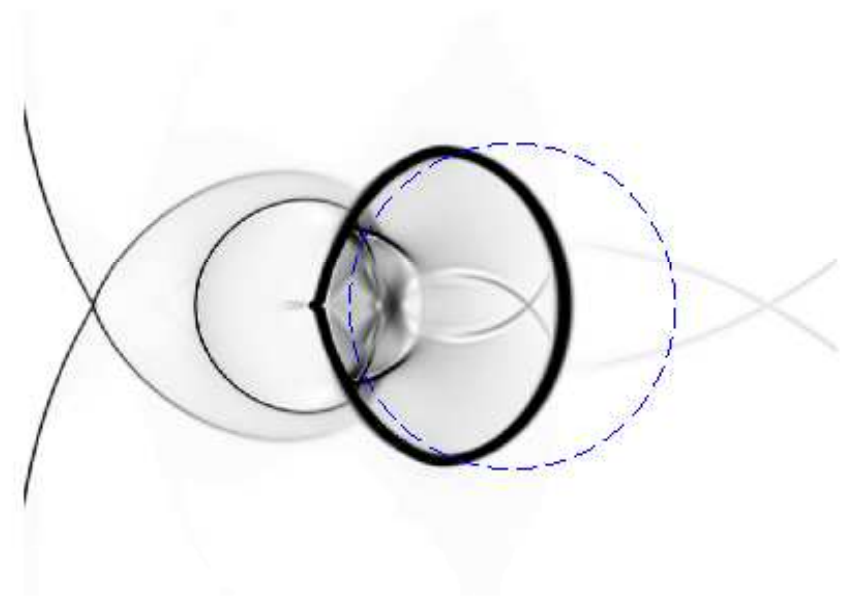
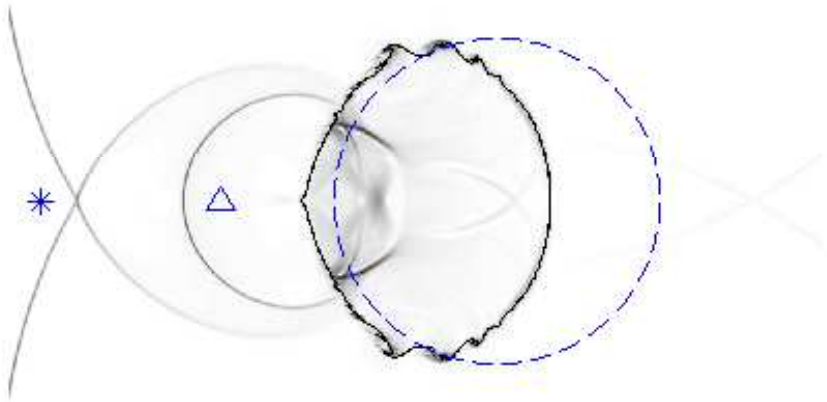
time = 187 μ s



Shock-Bubble Interaction Problem



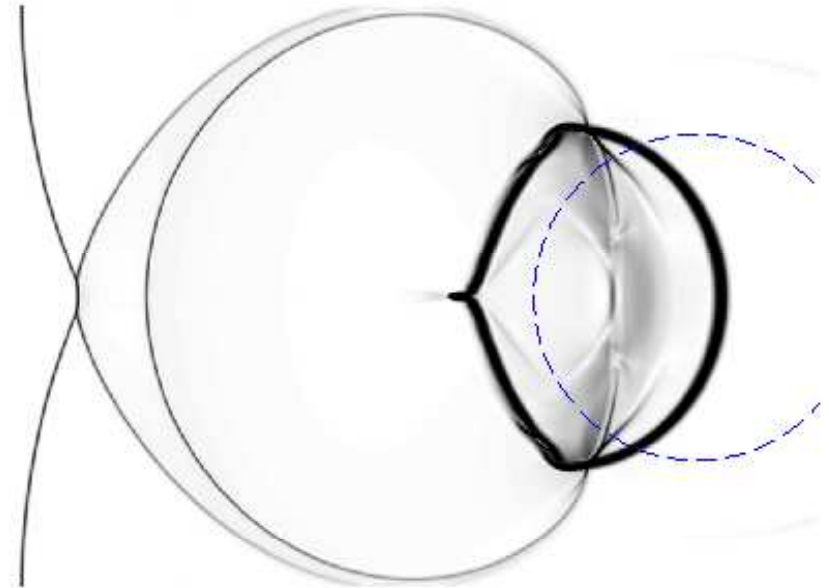
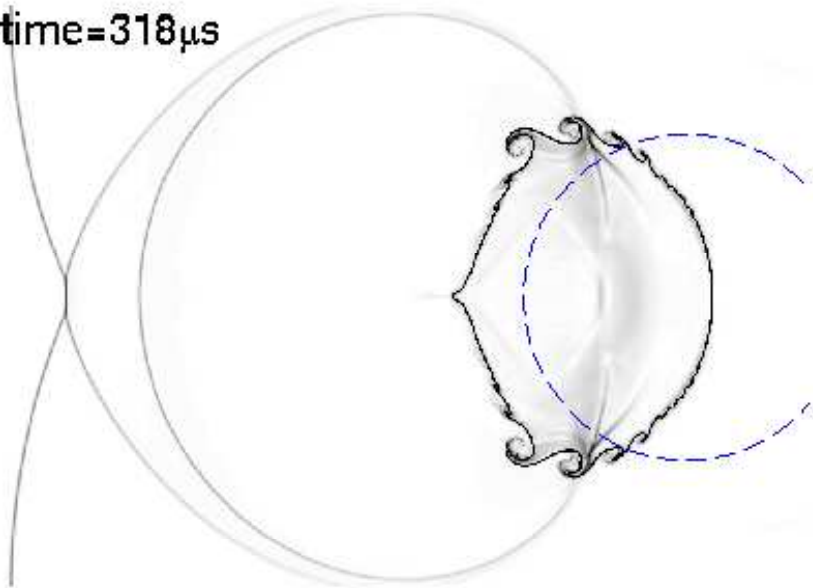
time=247 μ s



Shock-Bubble Interaction Problem



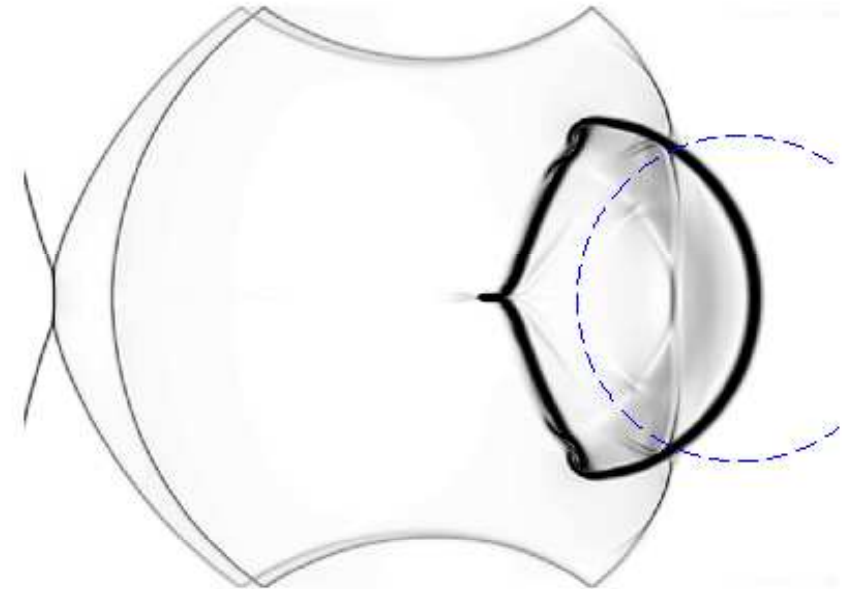
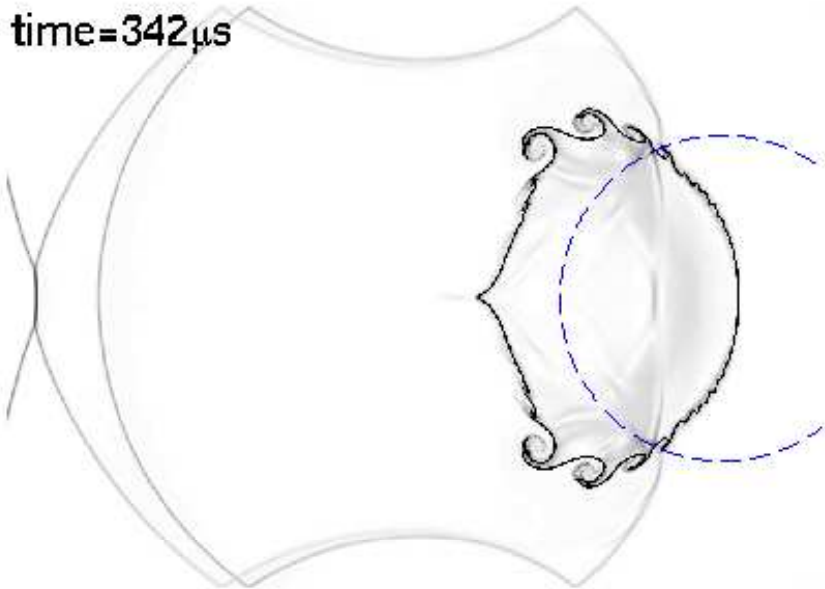
time=318 μ s



Shock-Bubble Interaction Problem



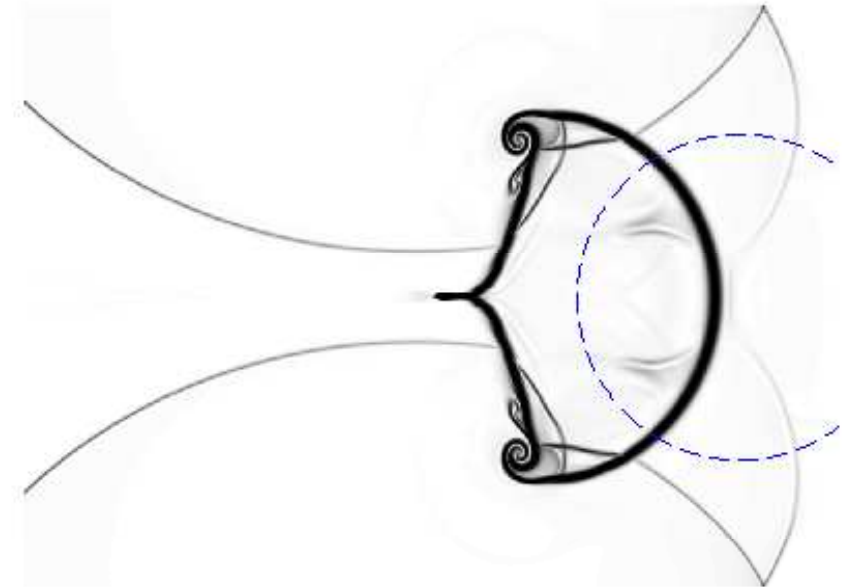
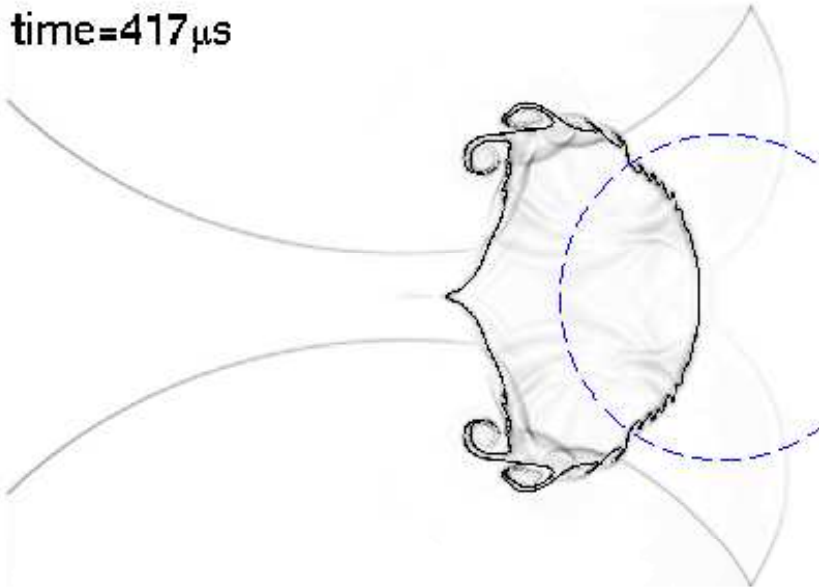
time=342 μ s



Shock-Bubble Interaction Problem



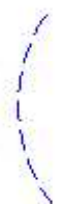
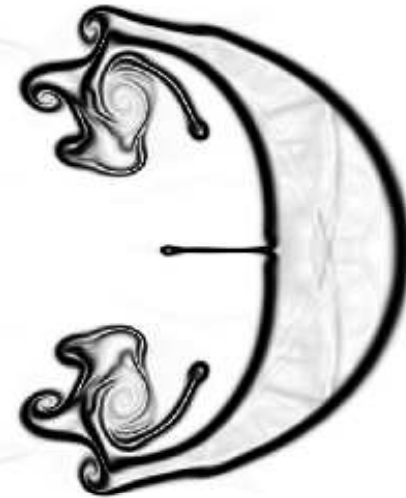
time=417 μ s



Shock-Bubble Interaction Problem



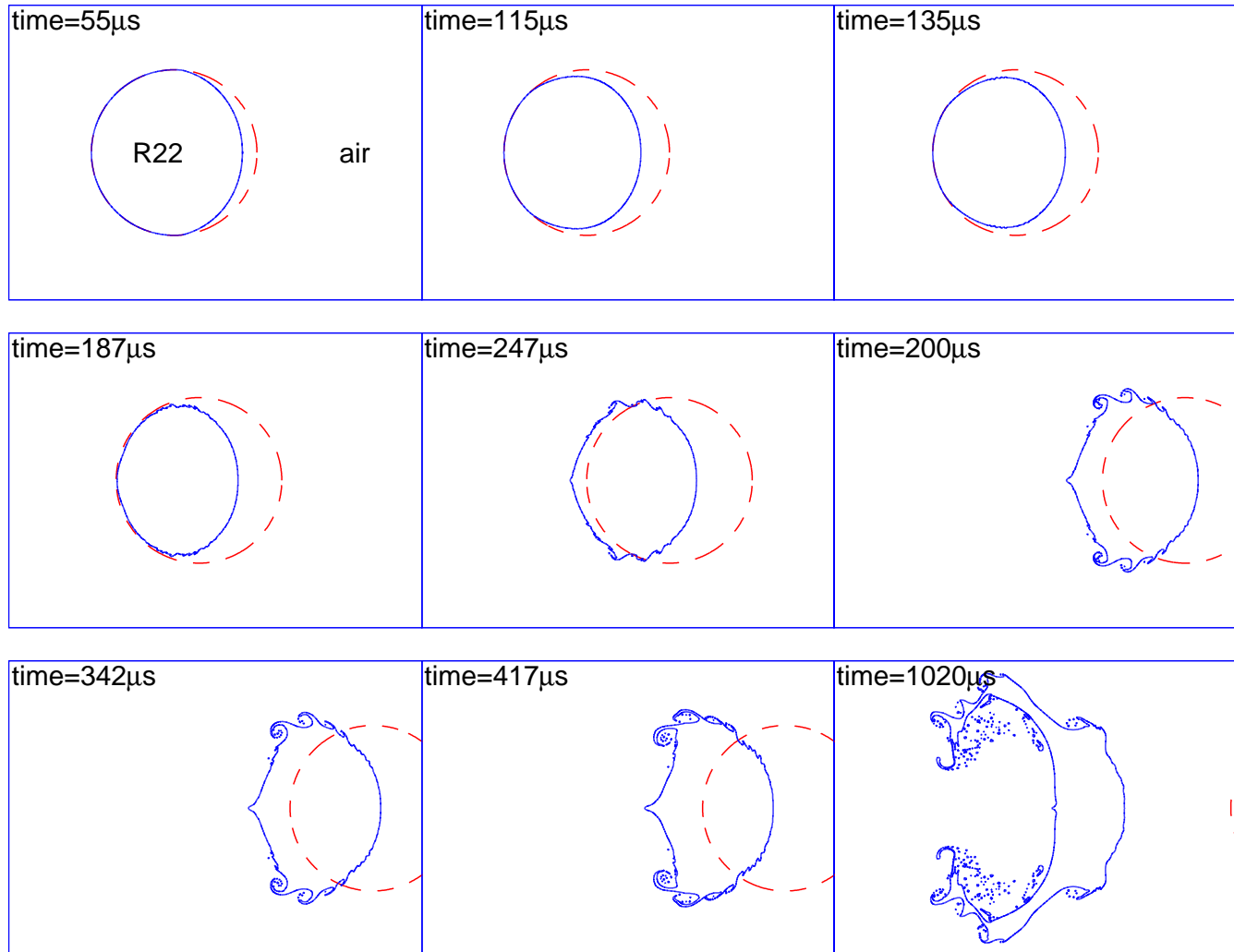
time = 1020 μ s



Shock-Bubble Interaction (cont.)



- Approximate locations of interfaces



Shock-Bubble Interaction (cont.)

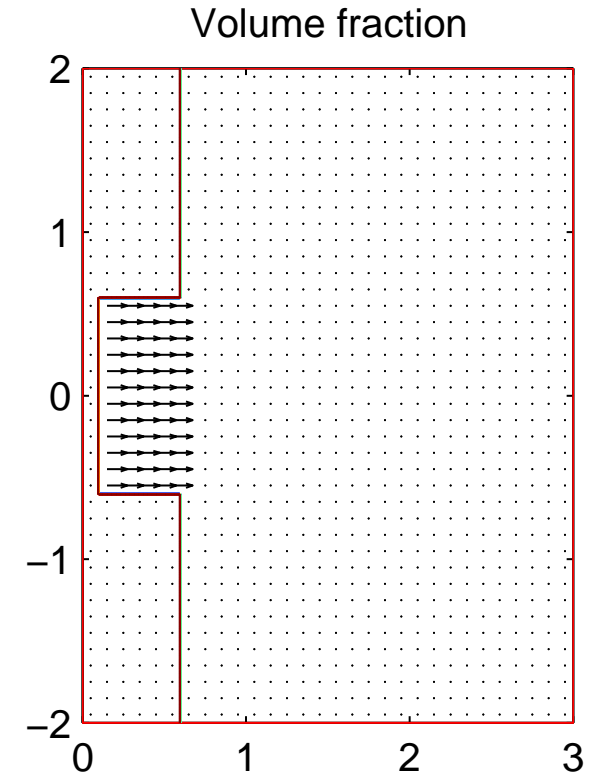
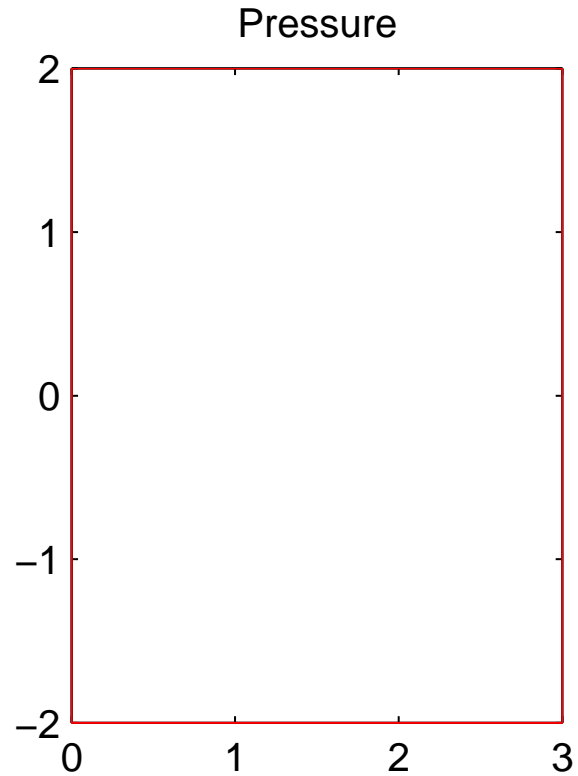
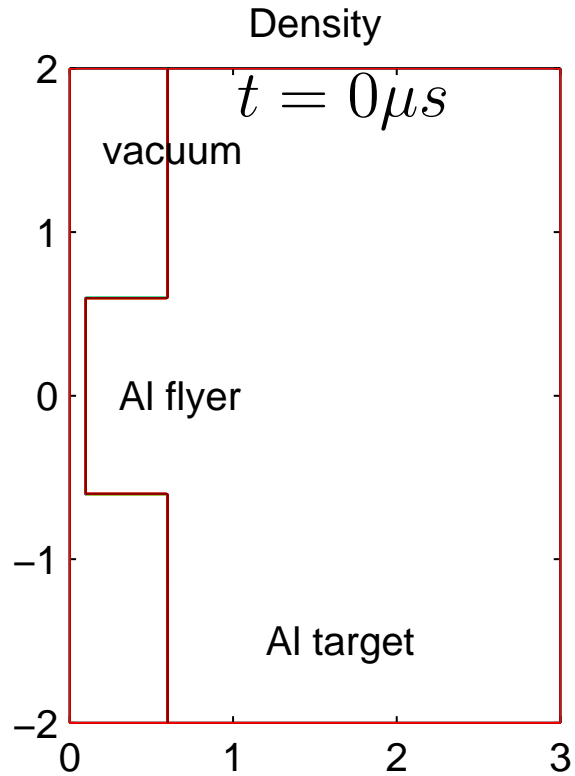


- Quantitative assessment of prominent flow velocities:

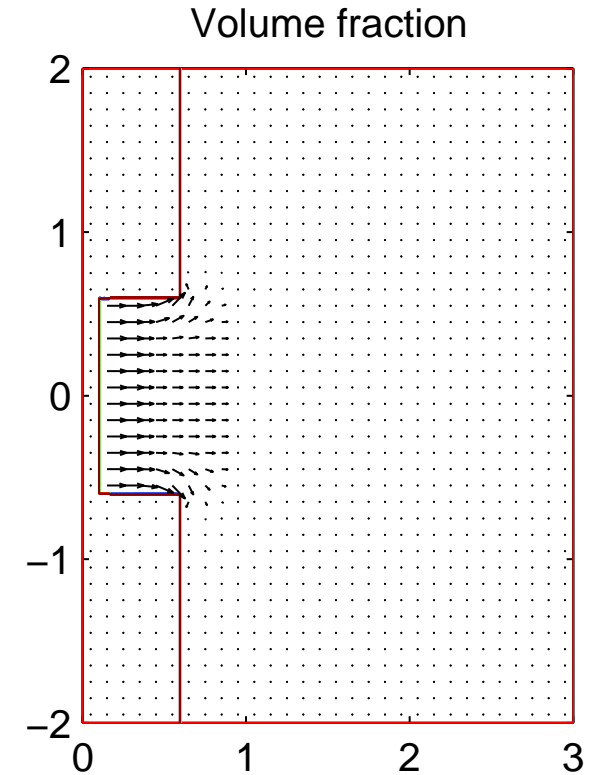
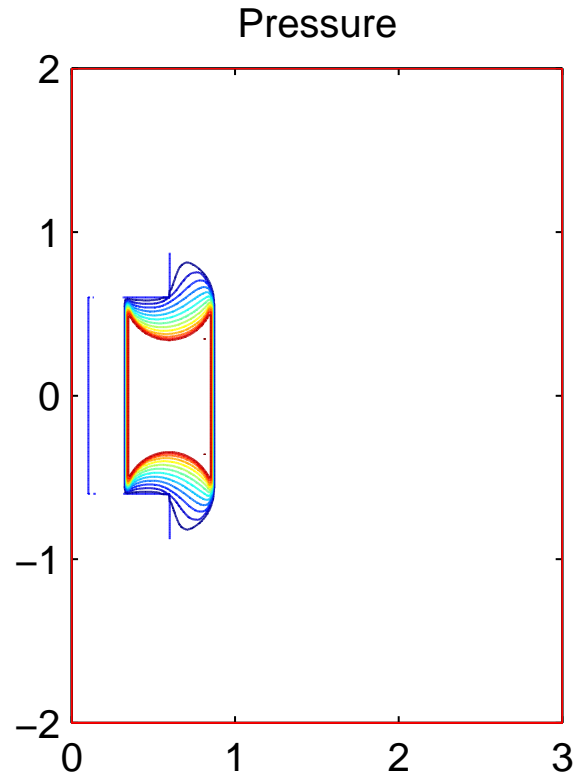
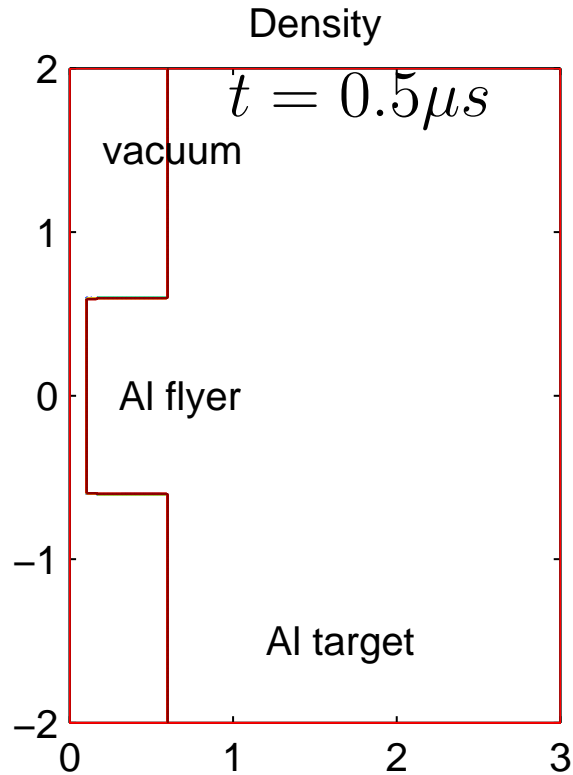
Velocity (m/s)	V_s	V_R	V_T	V_{ui}	V_{uf}	V_{di}	V_{df}
Haas & Sturtevant	415	240	540	73	90	78	78
Quirk & Karni	420	254	560	74	90	116	82
Our result (tracking)	411	243	538	64	87	82	60
Our result (capturing)	411	244	534	65	86	98	76

- V_s (V_R , V_T) **Incident (refracted, transmitted) shock speed** $t \in [0, 250]\mu\text{s}$ ($t \in [0, 202]\mu\text{s}$, $t \in [202, 250]\mu\text{s}$)
- V_{ui} (V_{uf}) **Initial (final) upstream bubble wall speed** $t \in [0, 400]\mu\text{s}$ ($t \in [400, 1000]\mu\text{s}$)
- V_{di} (V_{df}) **Initial (final) downstream bubble wall speed** $t \in [200, 400]\mu\text{s}$ ($t \in [400, 1000]\mu\text{s}$)

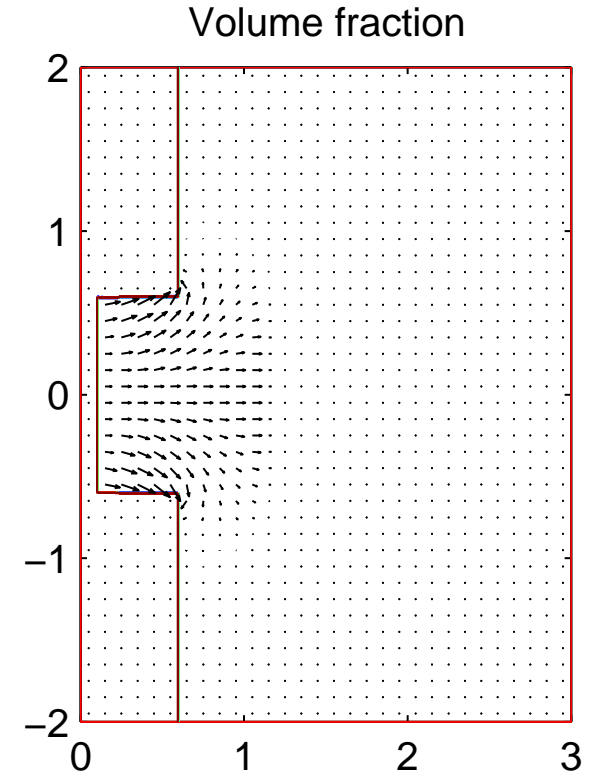
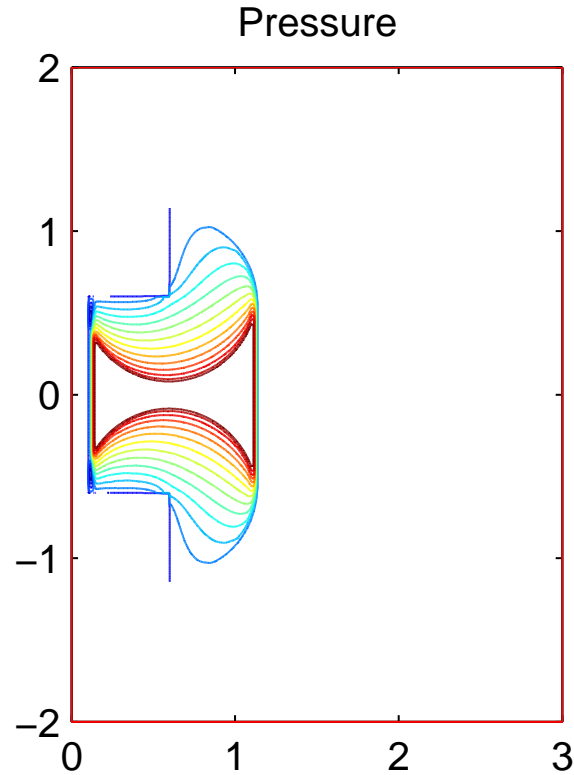
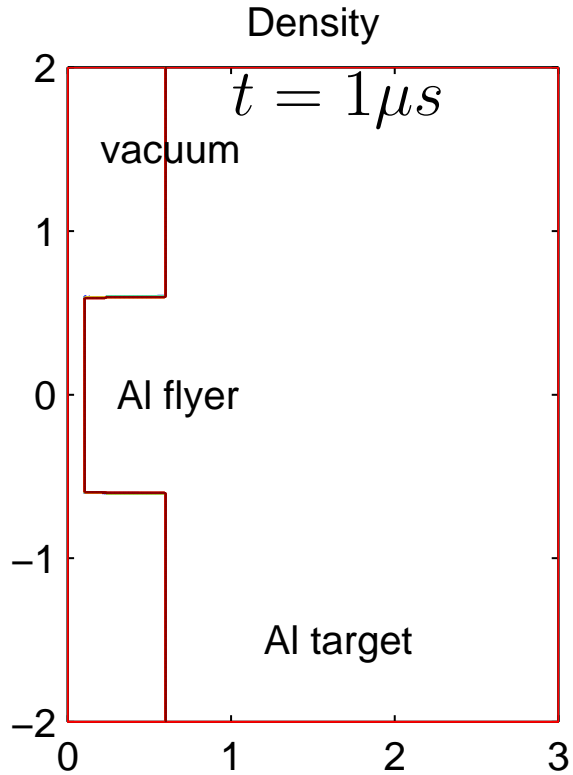
Aluminum-Plate Impact Problem



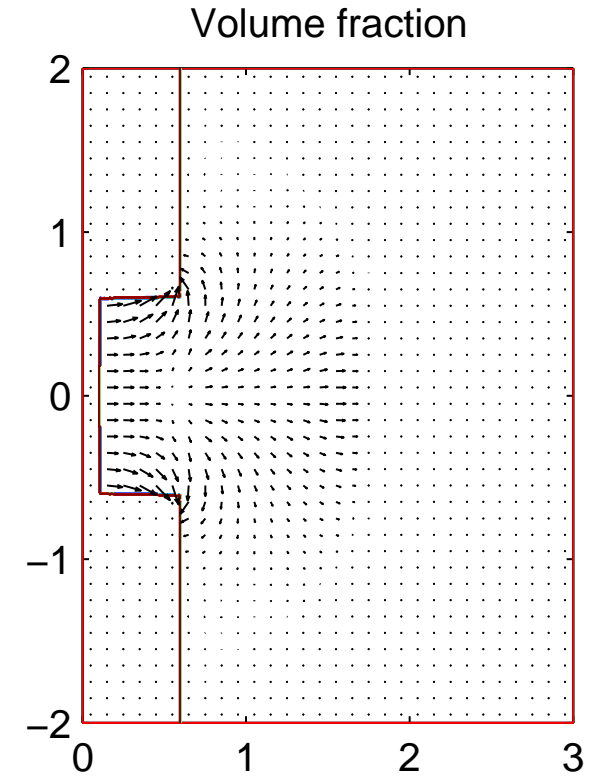
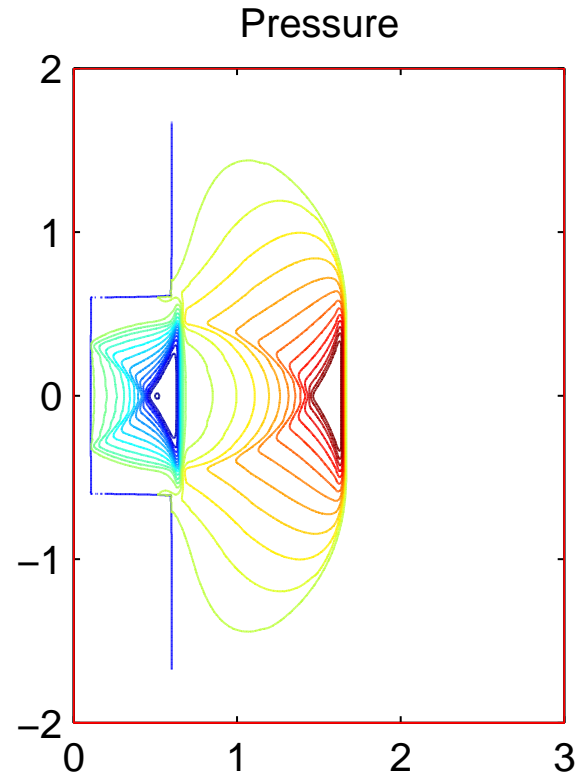
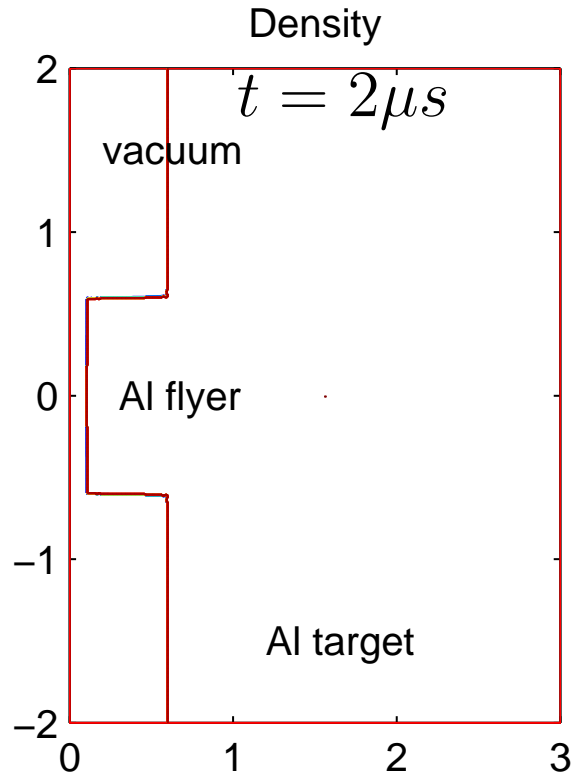
Aluminum-Plate Impact Problem



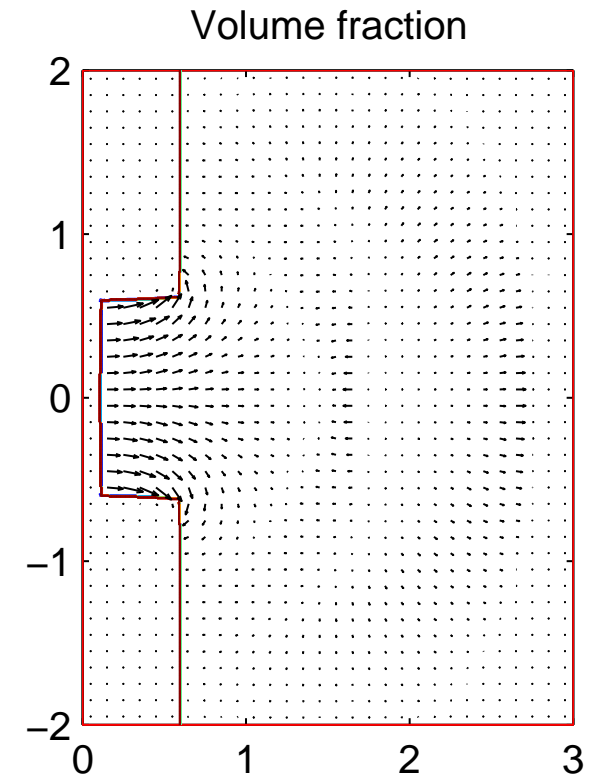
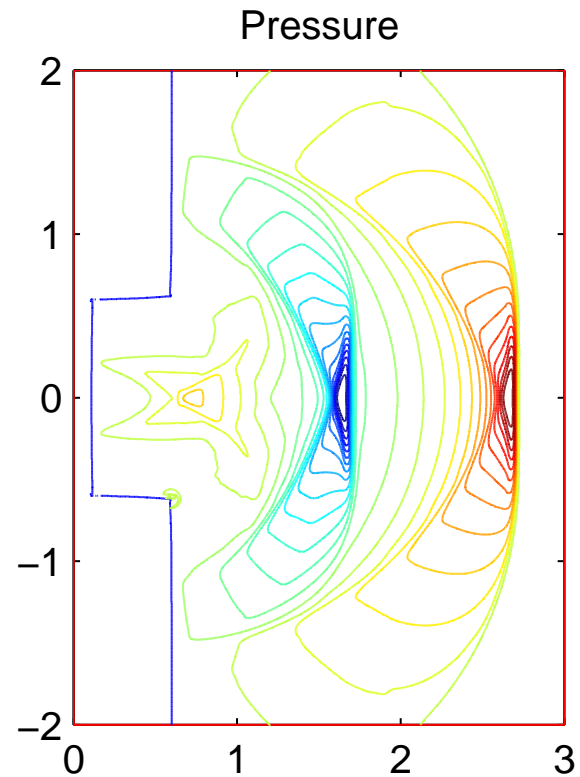
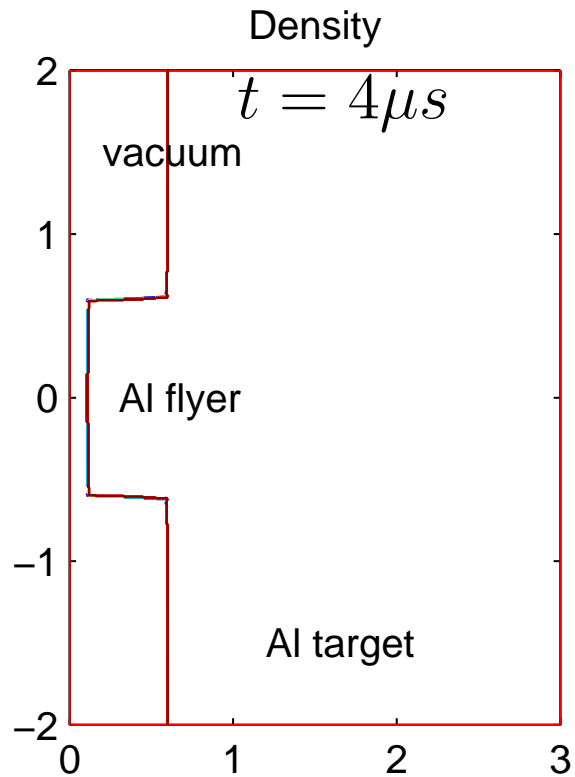
Aluminum-Plate Impact Problem



Aluminum-Plate Impact Problem



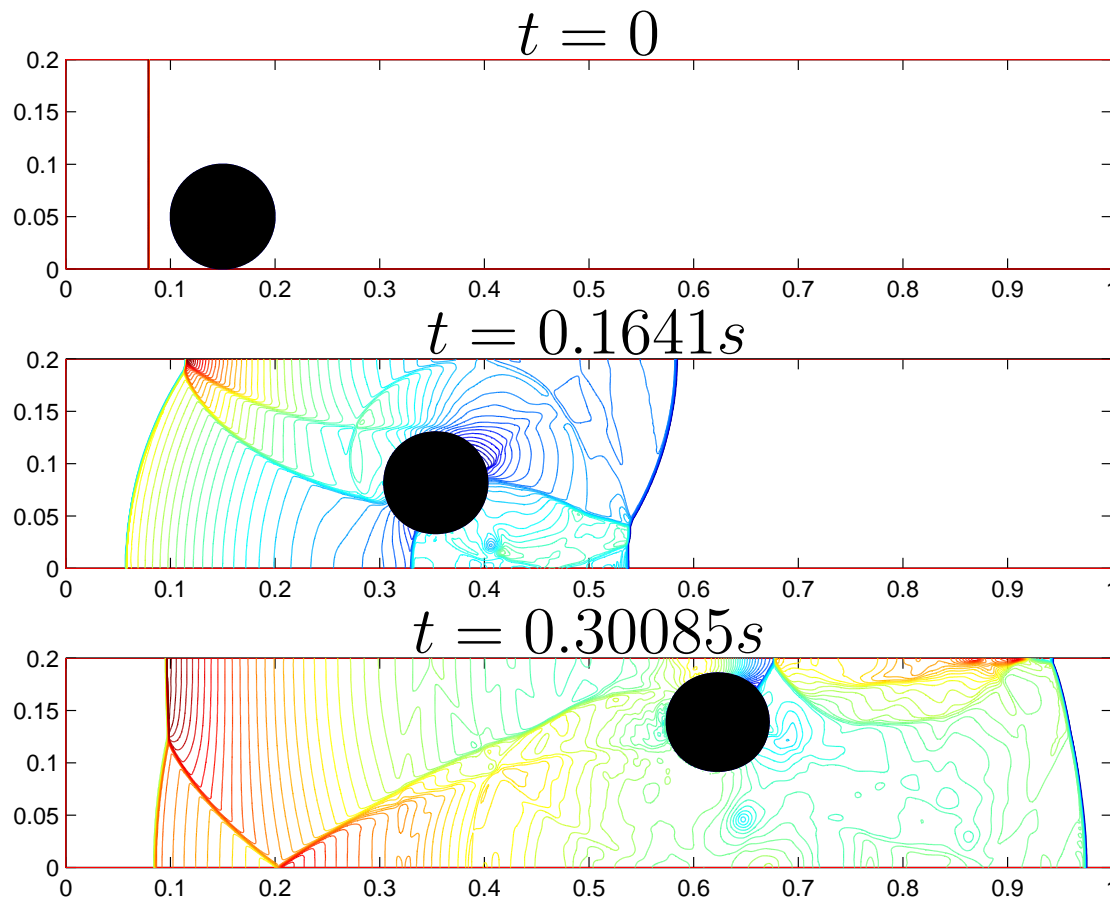
Aluminum-Plate Impact Problem



Cylinder lift-off Problem



- Moving speed of cylinder is governed by Newton's law
- Pressure contours are shown with a 1000×200 grid



Cylinder lift-off Problem

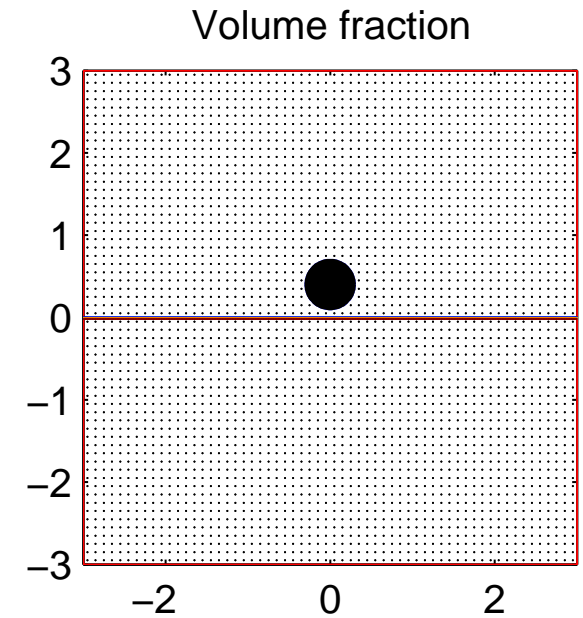
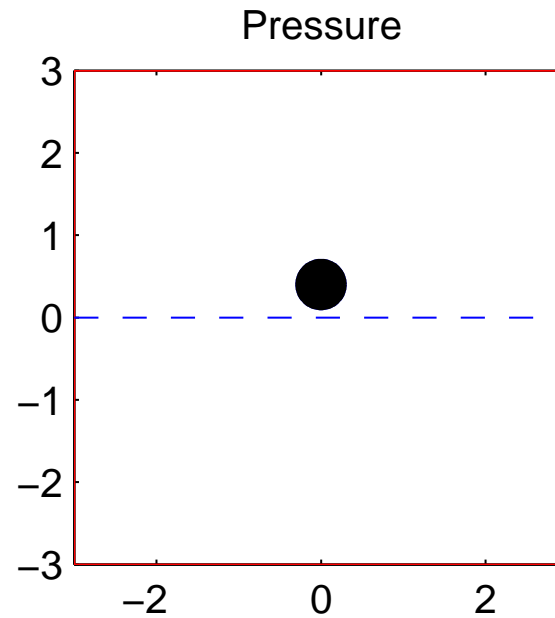
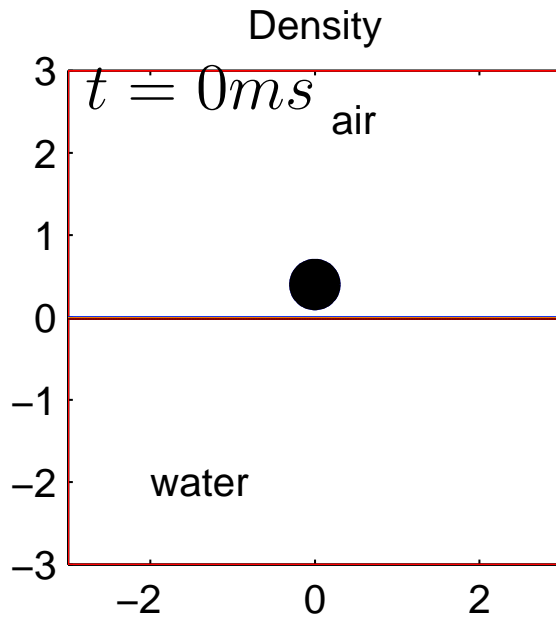


- A convergence study of center of cylinder & relative mass loss for at final stopping time $t = 0.30085s$

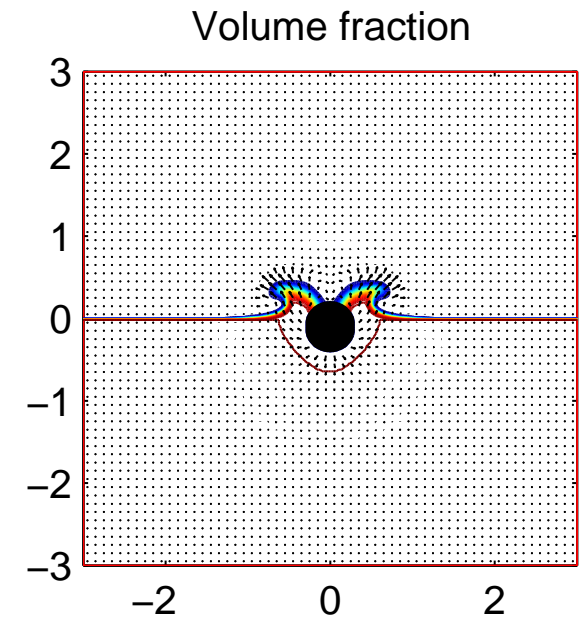
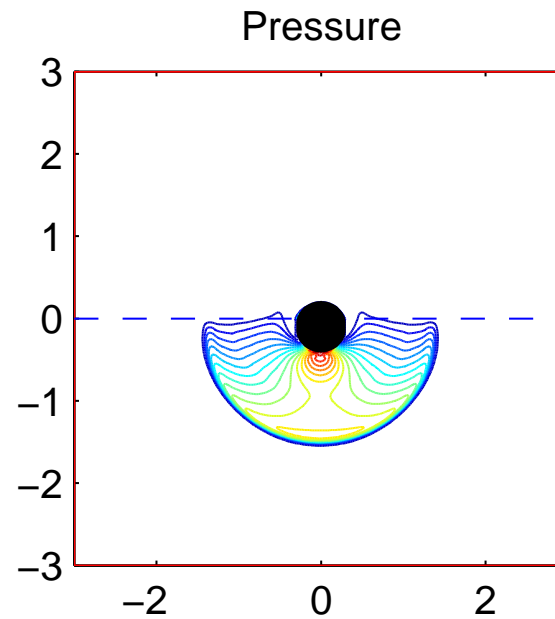
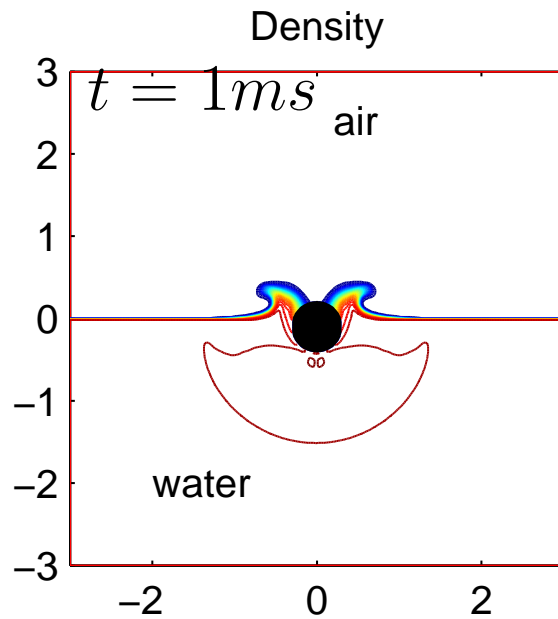
Mesh size	Center of cylinder	Relative mass loss
250×50	(0.618181, 0.134456)	-0.257528
500×100	(0.620266, 0.136807)	-0.131474
1000×200	(0.623075, 0.138929)	-0.066984

- Results are comparable with numerical appeared in literature

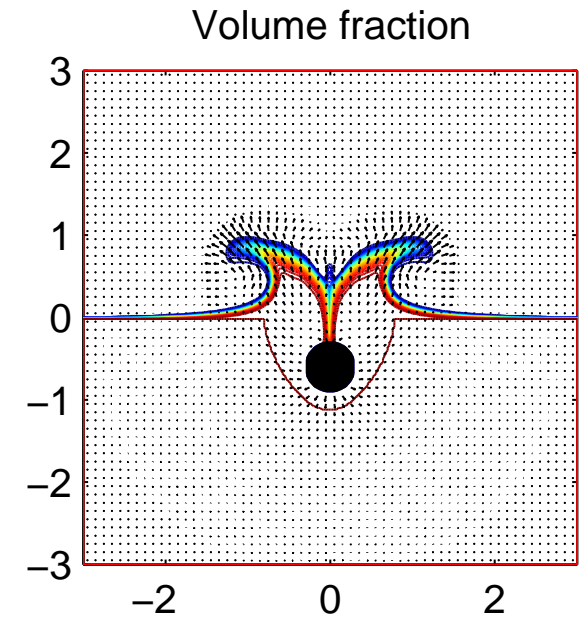
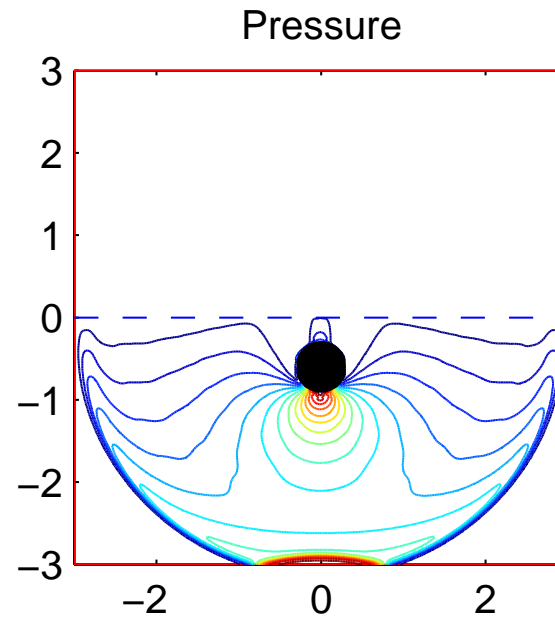
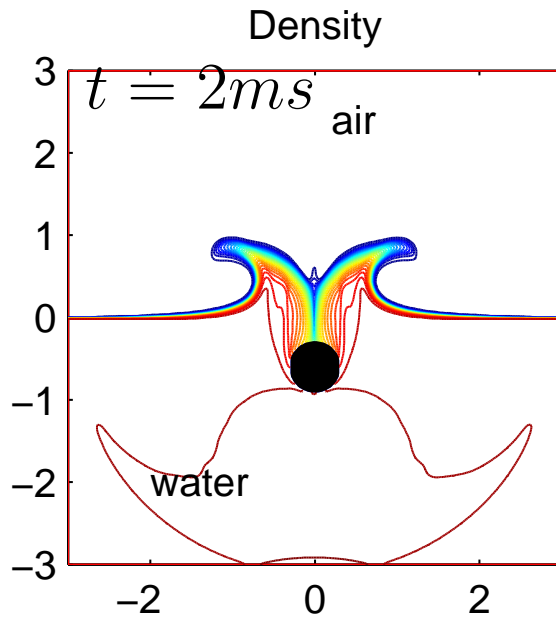
Falling Rigid Object in Water Tank



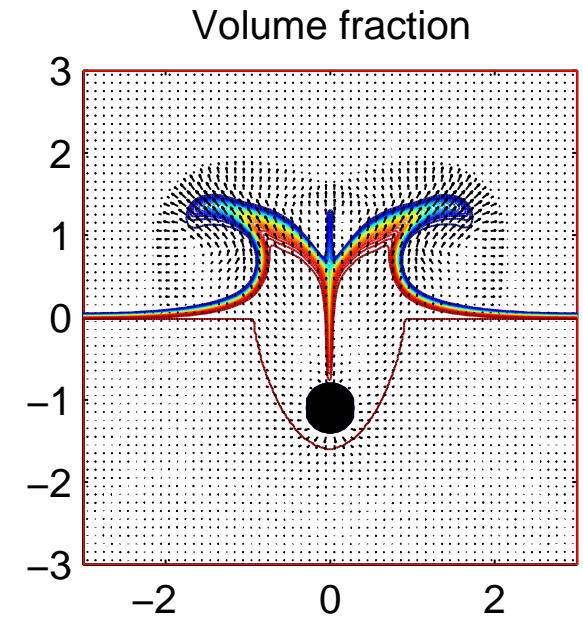
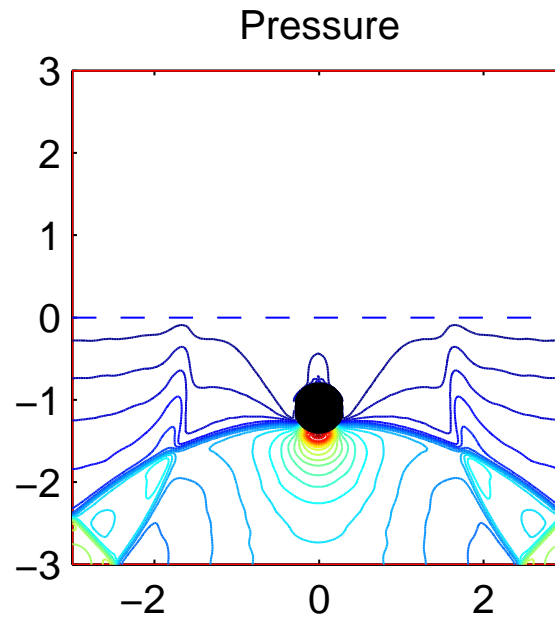
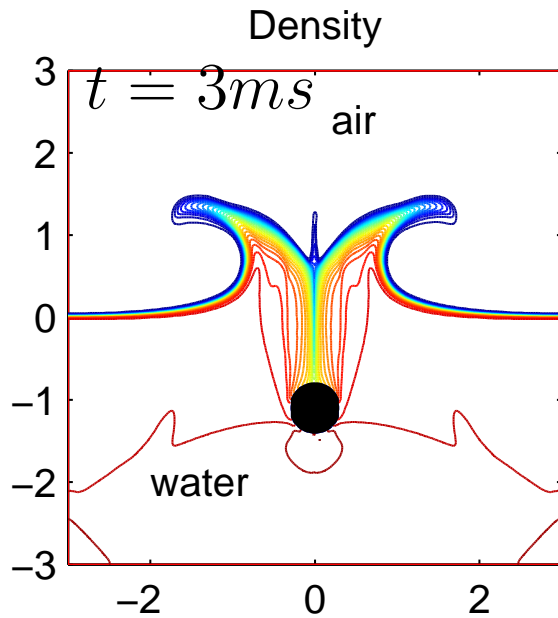
Falling Rigid Object in Water Tank



Falling Rigid Object in Water Tank



Falling Rigid Object in Water Tank



Future Work

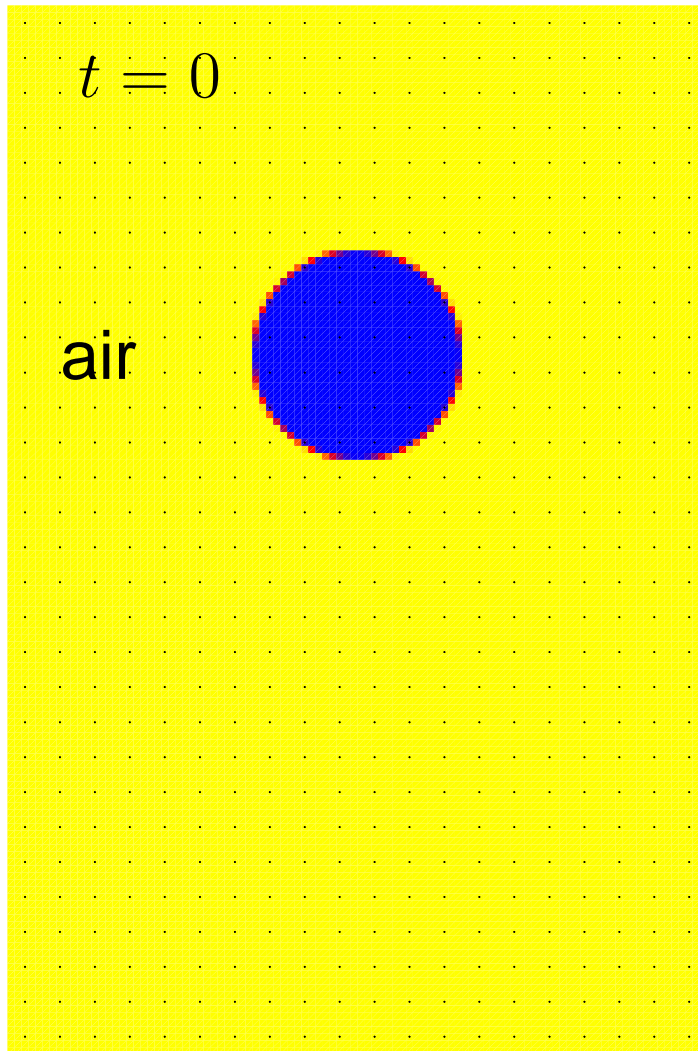


- 3D volume tracking method
- General curvilinear grid system
 - Body-fitted grid for complicated geometries
- Low Mach number flow
 - Remove sound-speed stiffness by preconditioning techniques or pressure-based method
- Include more physics towards real applications
 - Diffusion, phase transition, or elastic-plastic effect
- Hybrid surface-volume tracking algorithm for balance laws with interfaces & boundaries

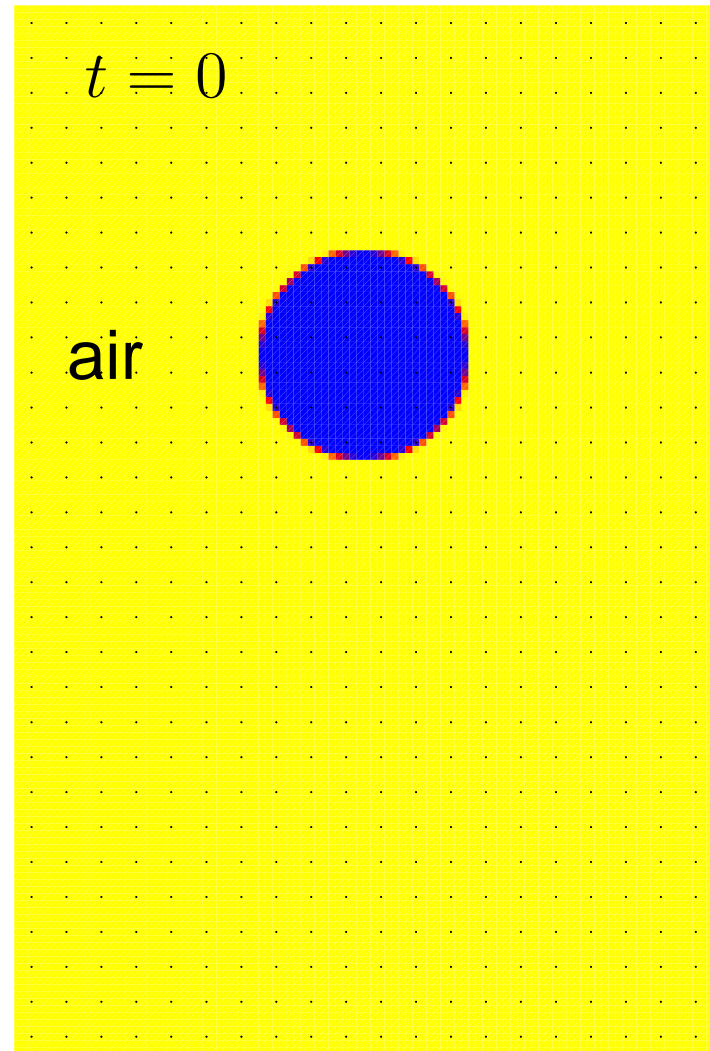
Liquid Drop Problem (Revisit)



Tracking



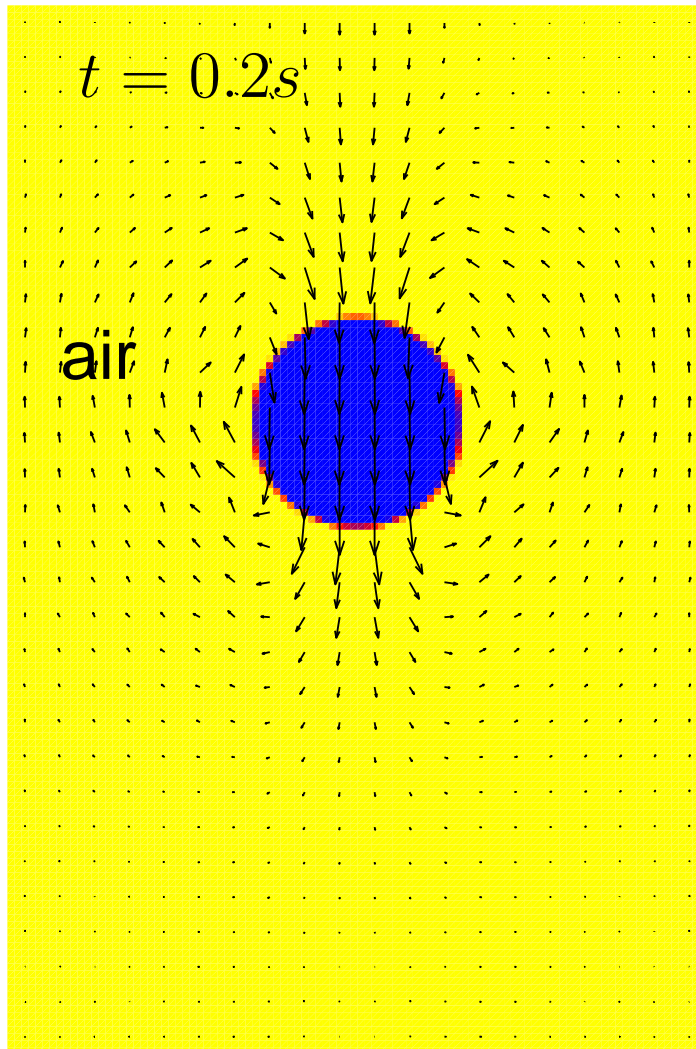
Capturing



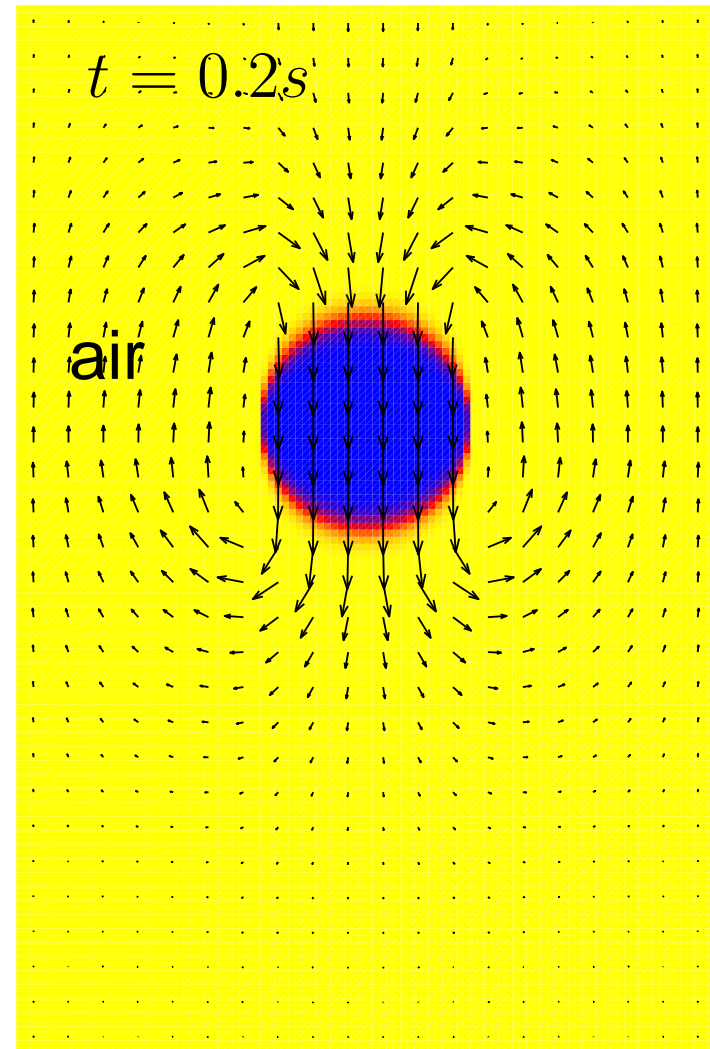
Liquid Drop Problem (Revisit)



Tracking



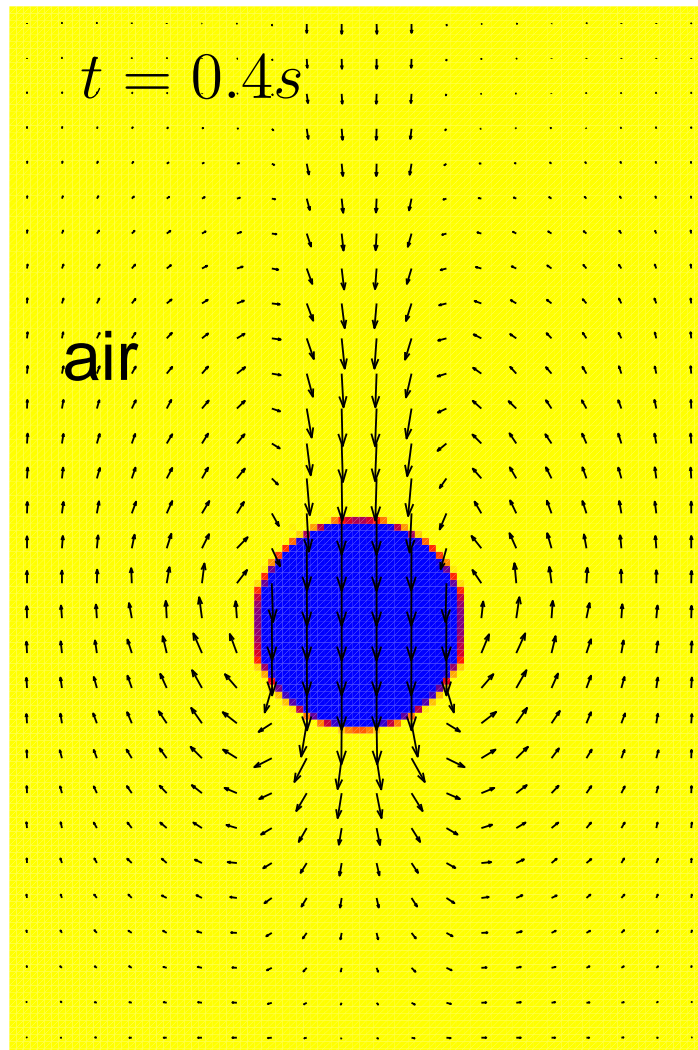
Capturing



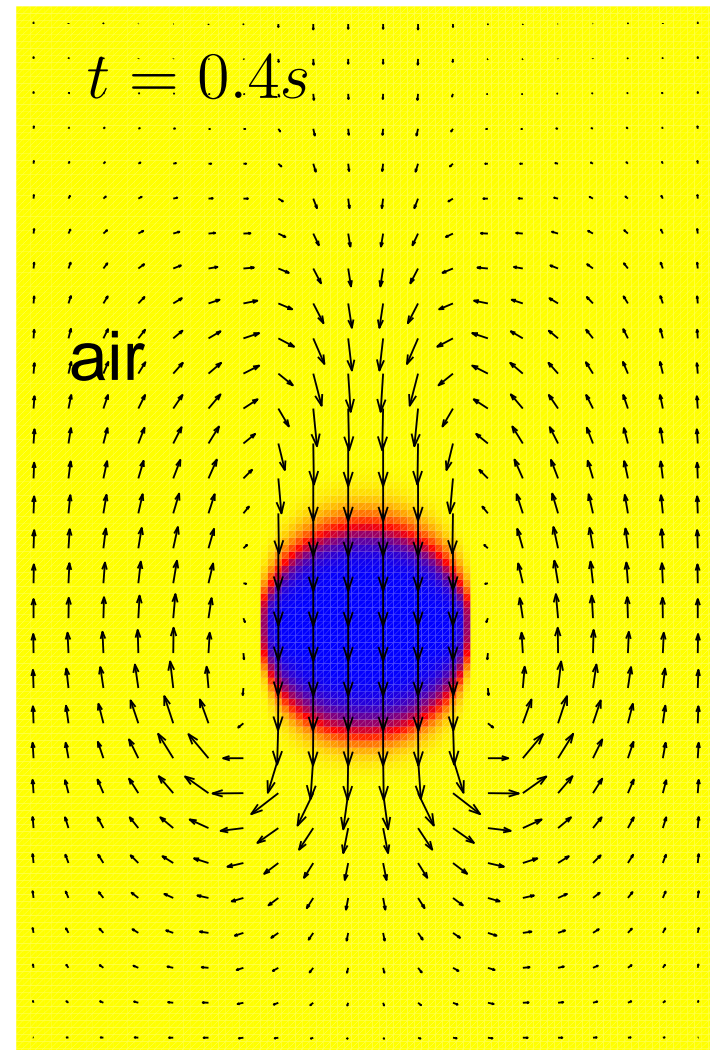
Liquid Drop Problem (Revisit)



Tracking



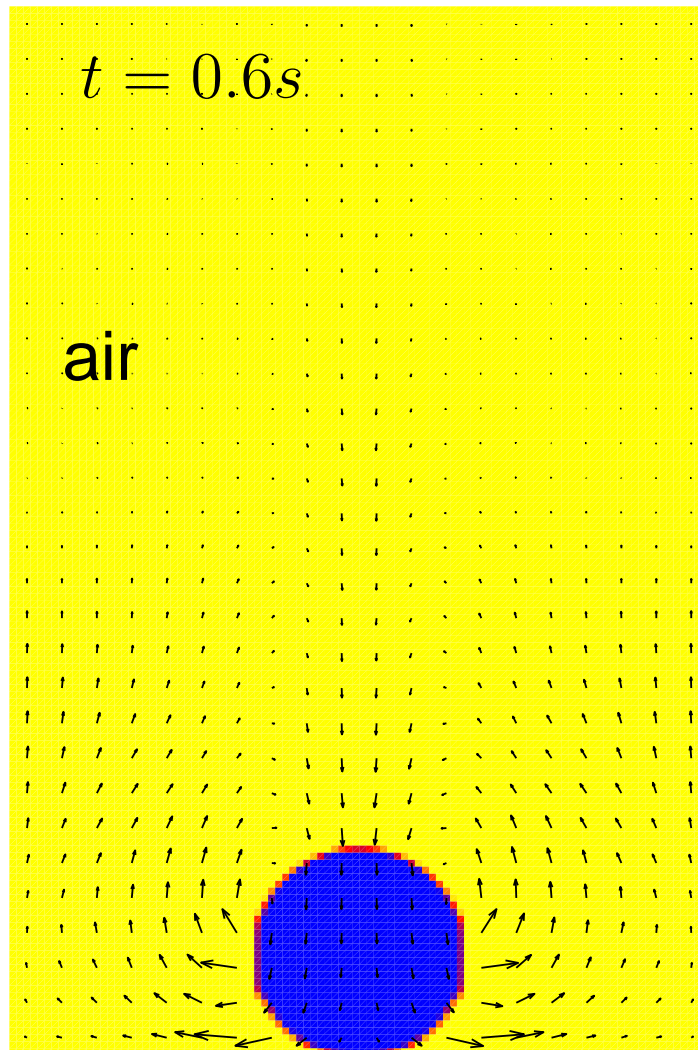
Capturing



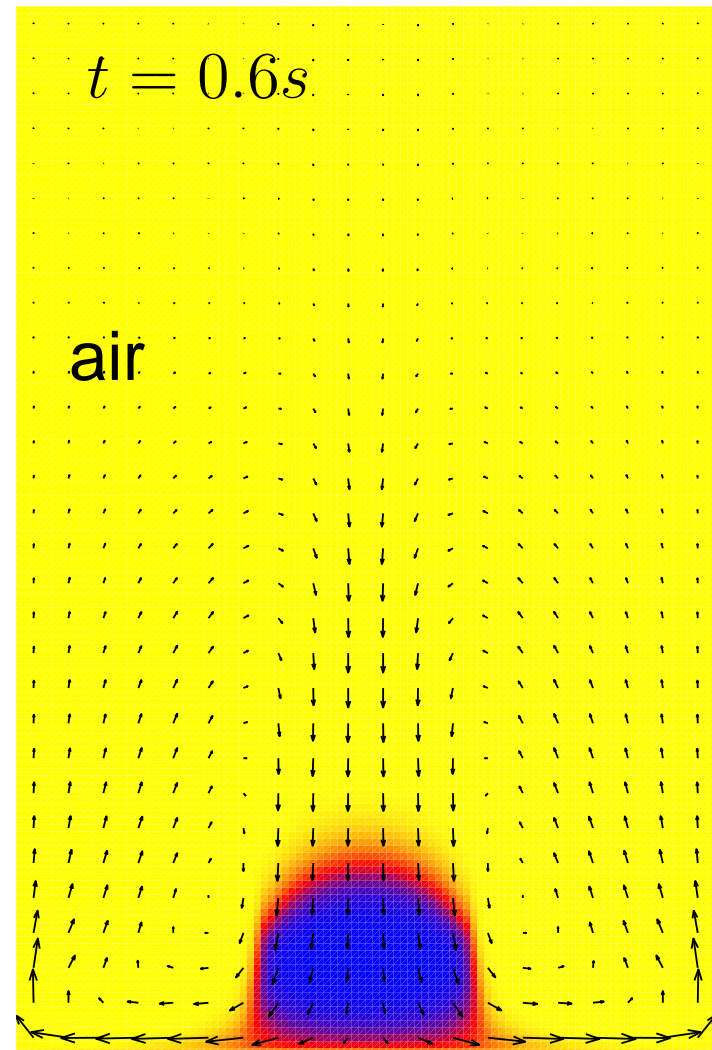
Liquid Drop Problem (Revisit)



Tracking



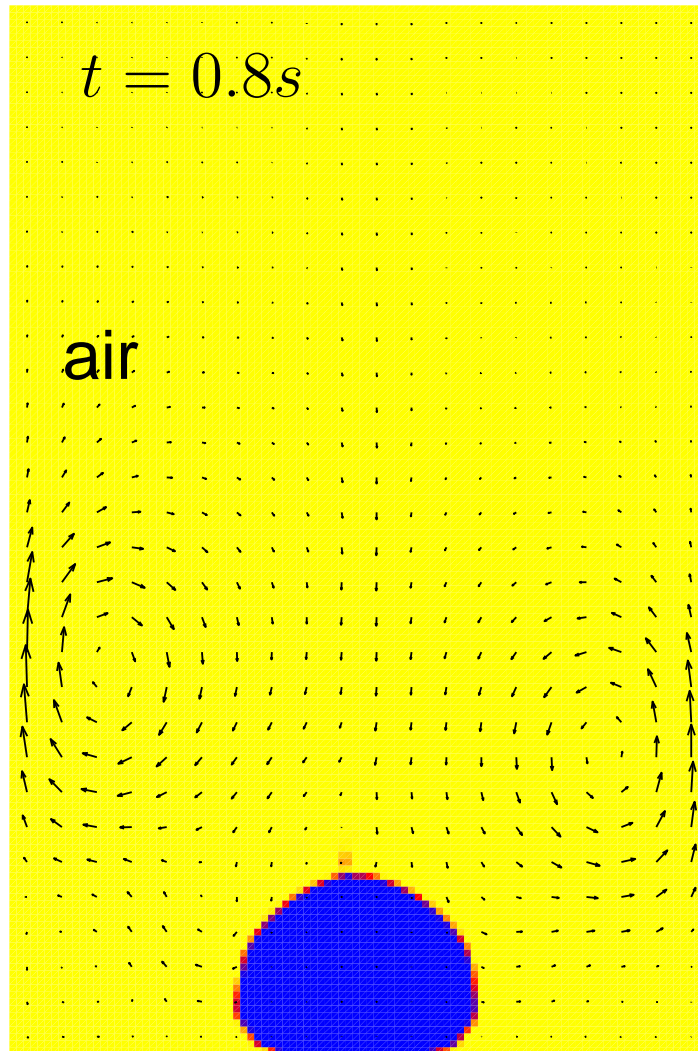
Capturing



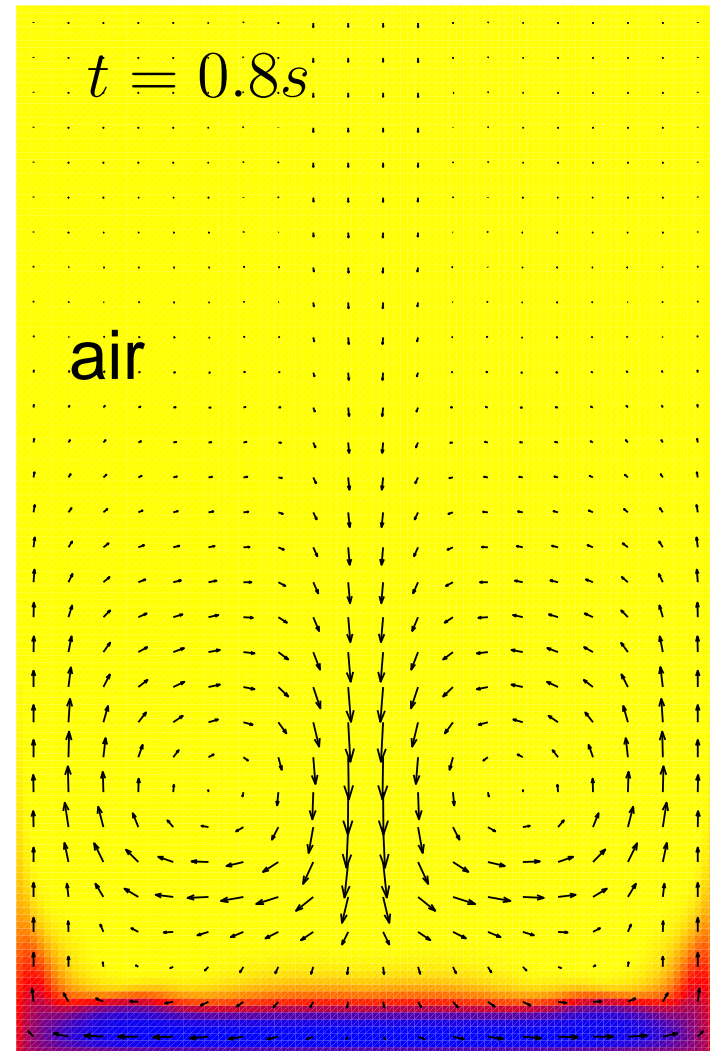
Liquid Drop Problem (Revisit)



Tracking



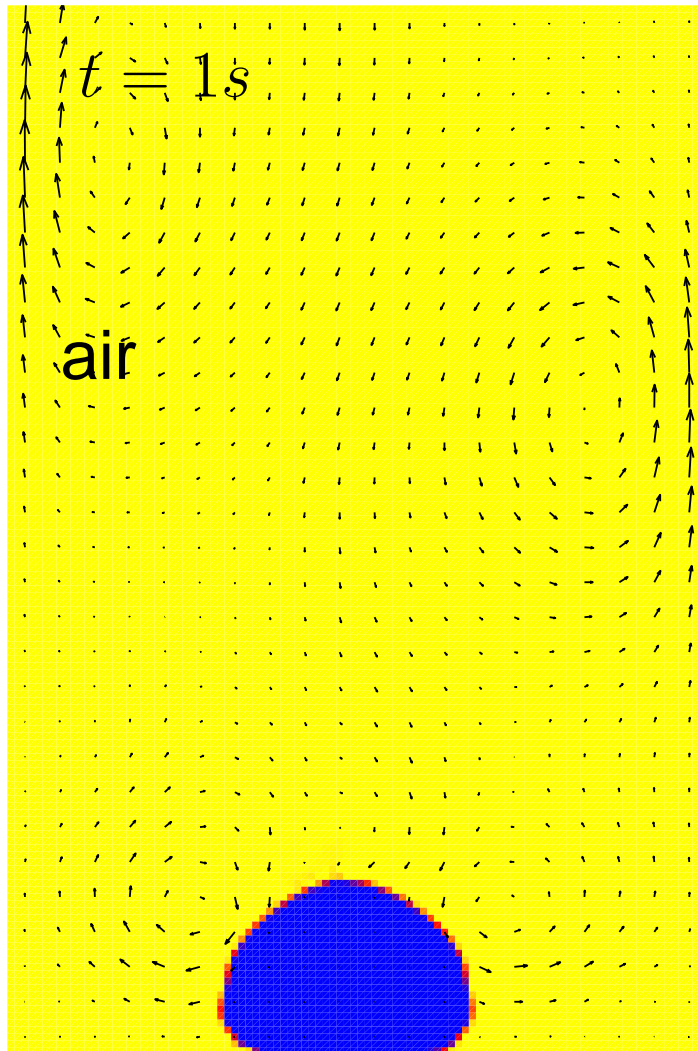
Capturing



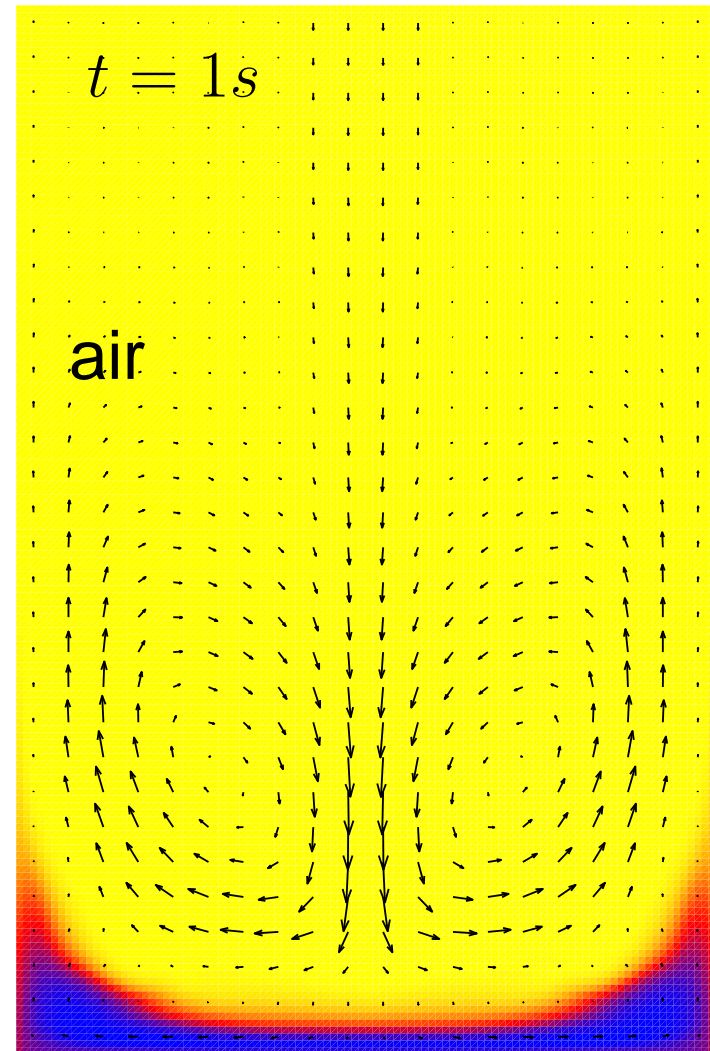
Liquid Drop Problem (Revisit)



Tracking



Capturing





Thank You

References



- (JCP 1998) An efficient shock-capturing algorithm for compressible multicomponent problems
- (JCP 1999, 2001) A fluid-mixture type algorithm for compressible multicomponent flow with **van der Waals (Mie-Grüneisen)** equation of state
- (JCP 2004) A fluid-mixture type algorithm for **barotropic** two-fluid flow Problems
- (JCP 2006) A wave-propagation based volume tracking method for compressible multicomponent flow in two space dimensions
- (Shock Waves 2006) A volume-fraction based algorithm for **hybrid barotropic & non-barotropic** two-fluid flow problems

Thermodynamic Stability



- Fundamental derivative of gas dynamics

$$\mathcal{G} = -\frac{V (\partial^2 p / \partial V^2)_S}{2 (\partial p / \partial V)_S}, \quad S : \text{specific entropy}$$

- Assume fluid state satisfy $\mathcal{G} > 0$ for thermodynamic stability, *i.e.*,

$$(\partial^2 p / \partial V^2)_S > 0 \quad \& \quad (\partial p / \partial V)_S < 0$$

- $(\partial^2 p / \partial V^2)_S > 0$ means **convex EOS**
- $(\partial p / \partial V)_S < 0$ means **real speed of sound**, for

$$c^2 = \left(\frac{\partial p}{\partial \rho} \right)_S = -V^2 \left(\frac{\partial p}{\partial V} \right)_S > 0$$

Homogeneous Flow Model (cont.)



- **Mie-Grüneisen EOS:** $p_k = p_{\text{ref}}(\rho_k) + \rho_k \Gamma(\rho_k) [e_k - e_{\text{ref}}(\rho_k)]$

$$\rho e = \sum_{k=1}^2 \alpha_k \rho_k e_k = \sum_{k=1}^2 \alpha_k \left[\frac{p - p_{\text{ref}}(\rho_k)}{\Gamma(\rho_k)} + \rho_k e_{\text{ref}}(\rho_k) \right] \quad \Rightarrow$$

$$p = \left[\rho e - \sum_{k=1}^2 \alpha_k \left(\frac{-p_{\text{ref}}(\rho_k)}{\Gamma(\rho_k)} + \rho_k e_{\text{ref}}(\rho_k) \right) \right]$$

Mie-Grüneisen Equations of State



- $(p_{\text{ref}}, e_{\text{ref}})$ lies along an **isentropo**e

1. **Jones-Wilkins-Lee** EOS for gaseous explosives

$$\Gamma(V) = \gamma - 1, \quad V = 1/\rho$$

$$e_{\text{ref}}(V) = e_0 + \frac{\mathcal{A} V_0}{\mathcal{R}_1} \exp\left(\frac{-\mathcal{R}_1 V}{V_0}\right) + \frac{\mathcal{B} V_0}{\mathcal{R}_2} \exp\left(\frac{-\mathcal{R}_2 V}{V_0}\right)$$

$$p_{\text{ref}}(V) = p_0 + \mathcal{A} \exp\left(\frac{-\mathcal{R}_1 V}{V_0}\right) + \mathcal{B} \exp\left(\frac{-\mathcal{R}_2 V}{V_0}\right)$$

2. **Cochran-Chan** EOS for solid explosives

$$\Gamma(V) = \gamma - 1$$

$$e_{\text{ref}}(V) = e_0 + \frac{-\mathcal{A} V_0}{1 - \mathcal{E}_1} \left[\left(\frac{V}{V_0}\right)^{1-\mathcal{E}_1} - 1 \right] + \frac{\mathcal{B} V_0}{1 - \mathcal{E}_2} \left[\left(\frac{V}{V_0}\right)^{1-\mathcal{E}_2} - 1 \right]$$

$$p_{\text{ref}}(V) = p_0 + \mathcal{A} \left(\frac{V}{V_0}\right)^{-\mathcal{E}_1} - \mathcal{B} \left(\frac{V}{V_0}\right)^{-\mathcal{E}_2}$$

Mie-Grüneisen EOS (cont.)



- $(p_{\text{ref}}, e_{\text{ref}})$ lies along a Hugoniot locus
 - Assume **linear** shock speed u_s & particle velocity u_p

$$u_s = c_0 + s u_p$$

- We may derive the relations

$$\Gamma(V) = \Gamma_0 \left(\frac{V}{V_0} \right)^\alpha, \quad \Gamma_0 = \gamma - 1$$

$$p_{\text{ref}}(V) = p_0 + \frac{c_0^2 (V_0 - V)}{[V_0 - s(V_0 - V)]^2}$$

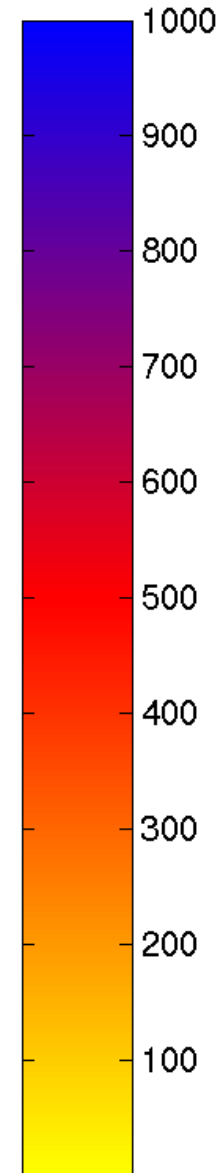
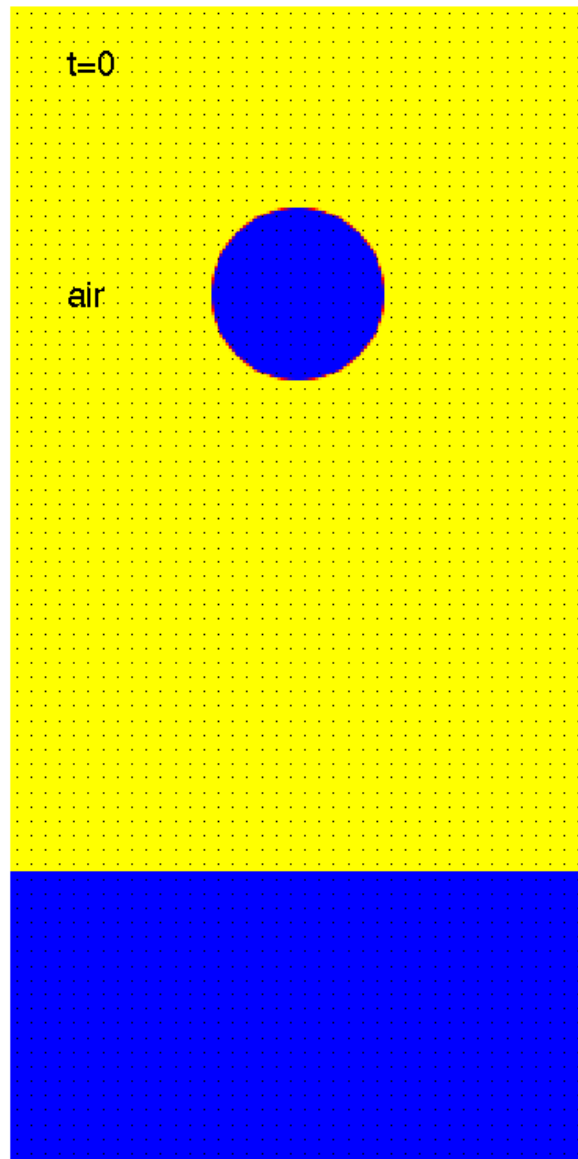
$$e_{\text{ref}}(V) = e_0 + \frac{1}{2} [p_{\text{ref}}(V) + p_0] (V_0 - V)$$

Material Quantities for Model EOS

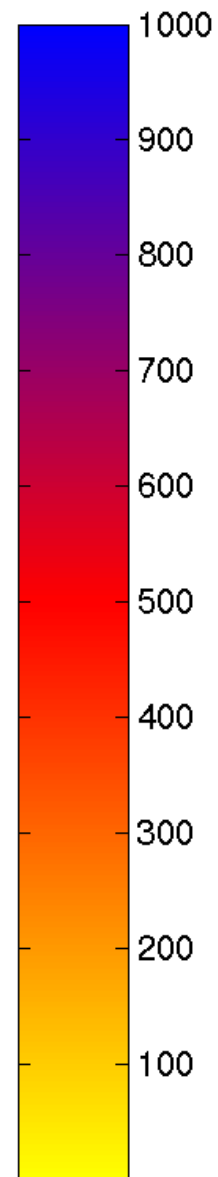
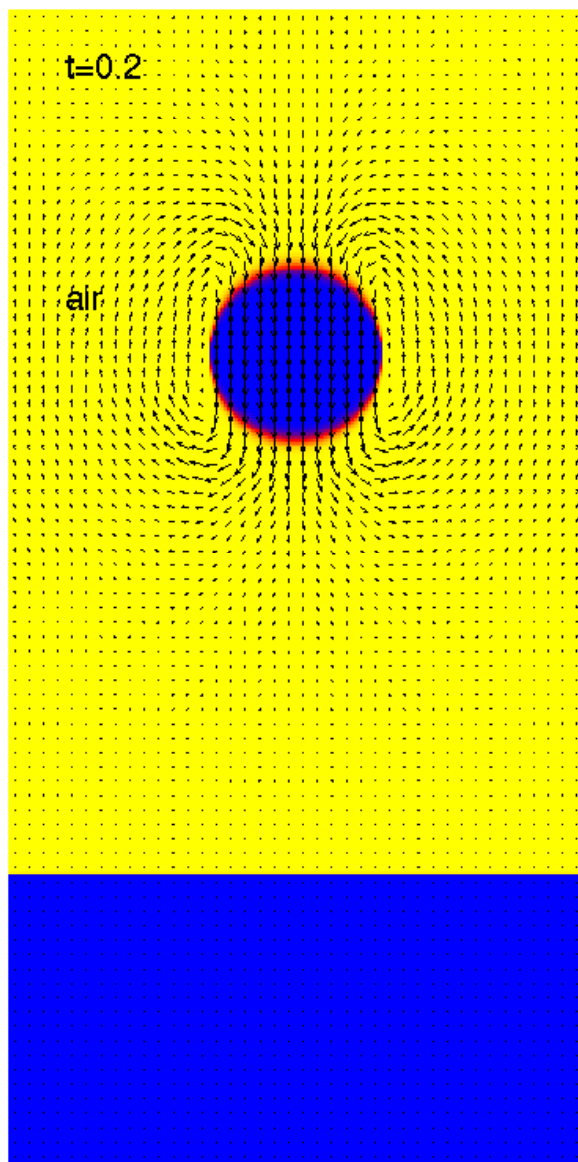


JWL EOS	$\rho_0(\text{kg/m}^3)$	$A(\text{GPa})$	$B(\text{GPa})$	\mathcal{R}_1	\mathcal{R}_2	Γ
TNT1	1630	371.2	3.23	4.15	0.95	0.30
TNT2	1630	548.4	9.375	4.94	1.21	1.28
Water	1004	1582	-4.67	8.94	1.45	1.17
CC EOS	$\rho_0(\text{kg/m}^3)$	$A(\text{GPa})$	$B(\text{GPa})$	\mathcal{E}_1	\mathcal{E}_2	Γ
TNT	1840	12.87	13.42	4.1	3.1	0.93
Copper	8900	145.67	147.75	2.99	1.99	2
Shock EOS	$\rho_0(\text{kg/m}^3)$	$c_0(\text{m/s})$	s	Γ_0	α	
Aluminum	2785	5328	1.338	2.0	1	
Copper	8924	3910	1.51	1.96	1	
Molybdenum	9961	4770	1.43	2.56	1	
MORB	2660	2100	1.68	1.18	1	
Water	1000	1483	2.0	2.0	10^{-4}	

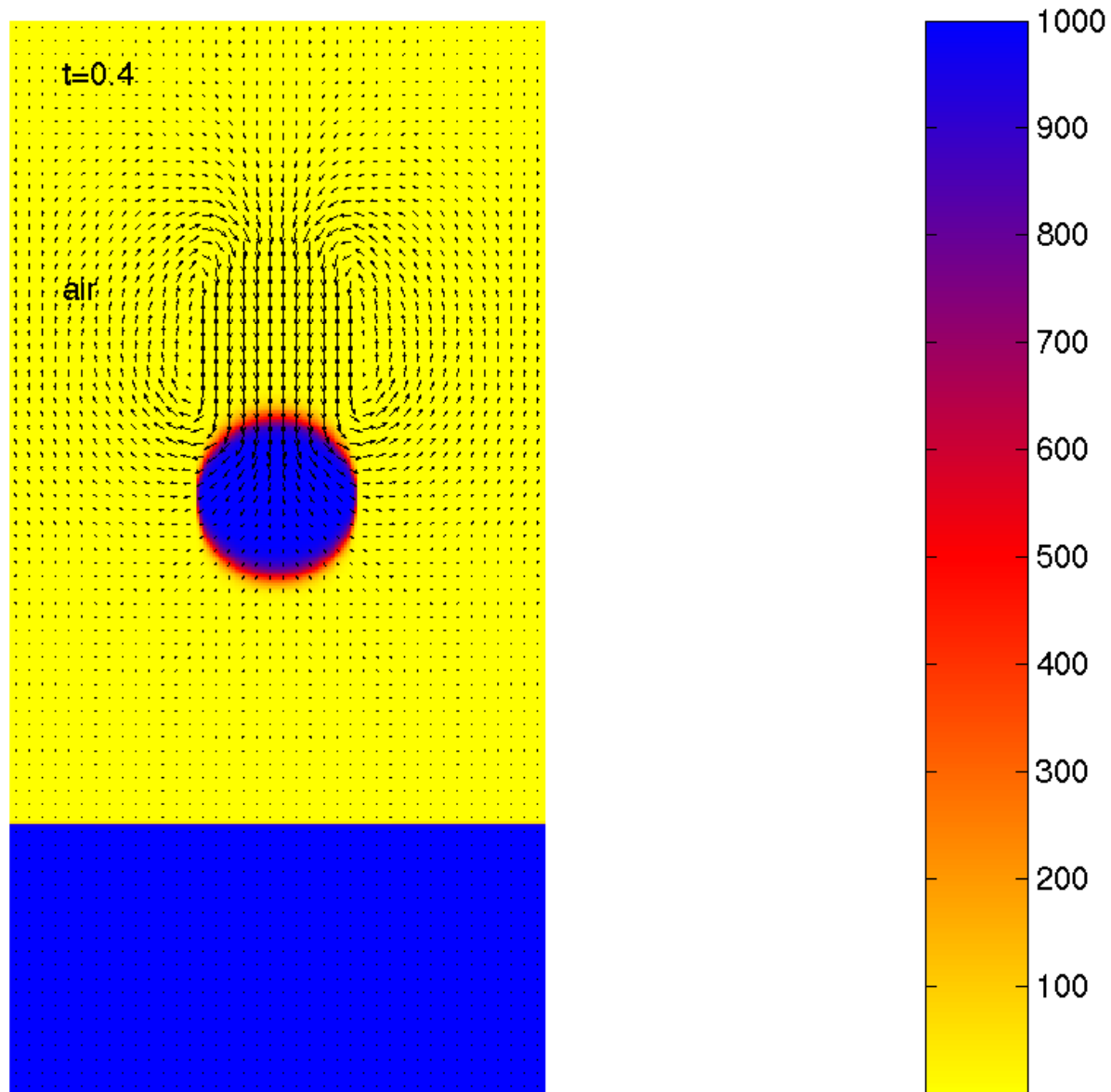
Falling Liquid Drop Problem



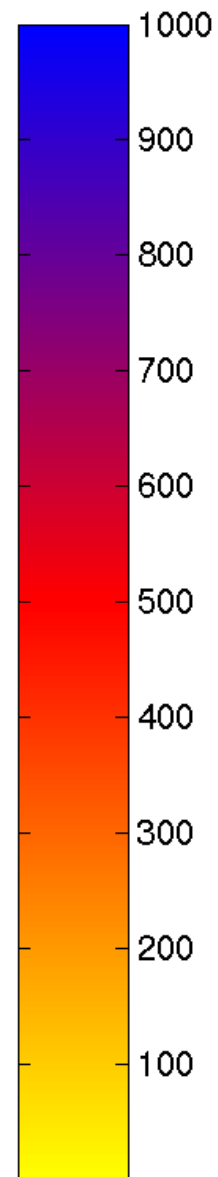
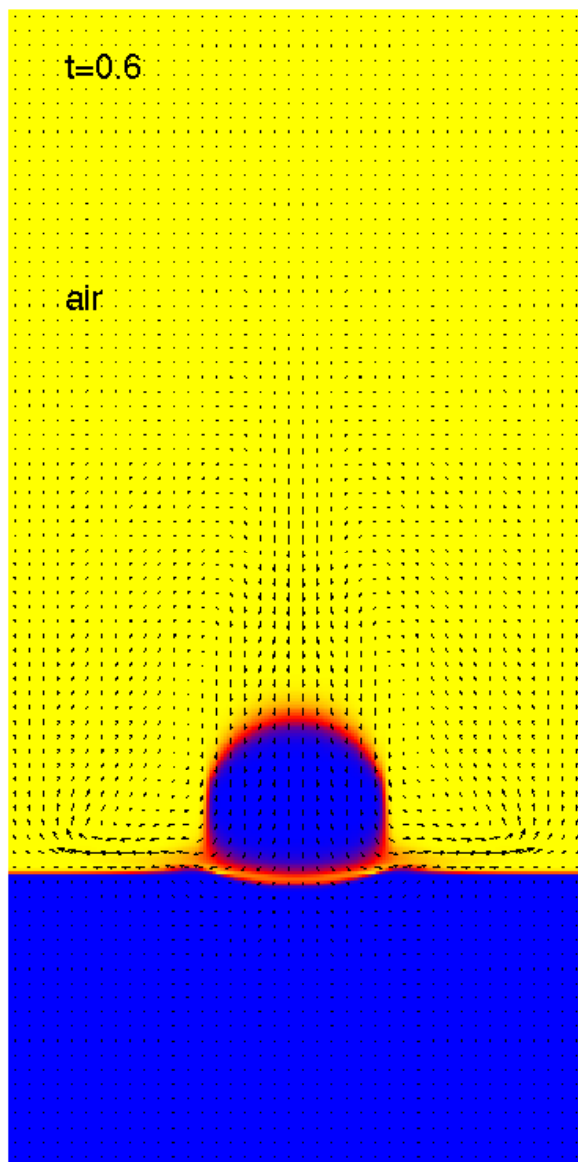
Falling Liquid Drop Problem



Falling Liquid Drop Problem



Falling Liquid Drop Problem



Falling Liquid Drop Problem

